

4/6/04

kam - 09 / 847048

Page 1

=> fil reg

FILE 'REGISTRY' ENTERED AT 10:53:29 ON 06 APR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 4 APR 2004 HIGHEST RN 671180-42-0
DICTIONARY FILE UPDATES: 4 APR 2004 HIGHEST RN 671180-42-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

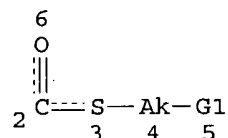
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que l29

L27 STR



VAR G1=CHO/N

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L29 9849 SEA FILE=REGISTRY SSS FUL L27

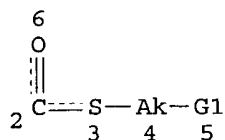
100.0% PROCESSED 122800 ITERATIONS

9849 ANSWERS

SEARCH TIME: 00.00.05

=> d que l30

L12	3379	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	23290/RID
L17	3476	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L12 OR ?VANCOMYCIN?/CNS
L18	97	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L17 NOT L12
L19	96	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L18 NOT CCS/CI
L20	40	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L19 NOT SQL/FA
L21	36	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L20 NOT ?TRANSFERASE?/CNS
L22	61	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L18 NOT L21
L23	3415	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	L17 NOT L22
L27						STR

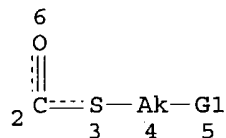


VAR G1=CHO/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE
L29 9849 SEA FILE=REGISTRY SSS FUL L27
L30 0 SEA FILE=REGISTRY ABB=ON PLU=ON L29 AND L23

=> d que l31
L27 STR

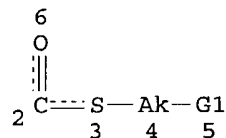


VAR G1=CHO/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE
L29 9849 SEA FILE=REGISTRY SSS FUL L27
L31 0 SEA FILE=REGISTRY ABB=ON PLU=ON L29 AND ?VANCOMYCIN?/CNS

=> d sta que l46
L27 STR



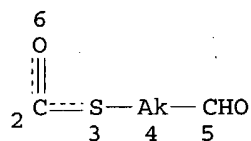
VAR G1=CHO/N
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L29 9849 SEA FILE=REGISTRY SSS FUL L27

L41 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L42 90 SEA FILE=REGISTRY SUB=L29 SSS FUL L41

L43 32 SEA FILE=REGISTRY ABB=ON PLU=ON L42 AND (C18H34OS2 OR C7H12OS2 OR C8H14O2S OR C13H16O2S OR C7H10O2S OR C5H8O2S OR C8H14O2S OR C9H16O2S OR C4H6O2S OR C12H12O2S OR C13H22O2S OR C6H10O2S OR C11H20O2S OR C11H12O2S OR C9H16O2S OR C12H14O2S OR C8H14O2S OR C13H24O2S OR C7H10O2S OR C5H6O2S OR C10H8O2S OR C17H16O2S)

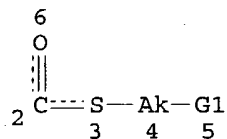
L44 58 SEA FILE=REGISTRY ABB=ON PLU=ON L42 NOT L43

L45 2 SEA FILE=REGISTRY ABB=ON PLU=ON L44 AND (C18H34O2S OR C7H12O2S)

L46 34 SEA FILE=REGISTRY ABB=ON PLU=ON (L43 OR L45)

=> d sta que 156

L27 STR



VAR G1=CHO/N

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

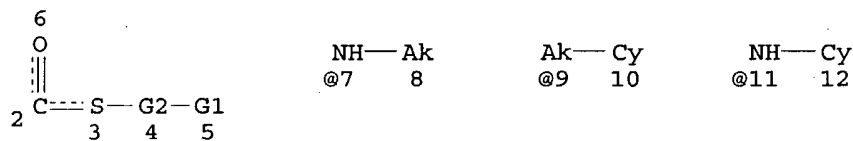
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L29 9849 SEA FILE=REGISTRY SSS FUL L27

L54 STR



VAR G1=NH2/7/11

VAR G2=AK/9

NODE ATTRIBUTES:

CONNECT IS M1 RC AT 2
CONNECT IS M1 RC AT 10
CONNECT IS M1 RC AT 12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L56 509 SEA FILE=REGISTRY SUB=L29 CSS FUL L54

100.0% PROCESSED 9780 ITERATIONS
SEARCH TIME: 00.00.01

509 ANSWERS

=> d his

(FILE 'HOME' ENTERED AT 09:40:00 ON 06 APR 2004)
SET COST OFF

FILE 'HCAPLUS' ENTERED AT 09:40:16 ON 06 APR 2004

E MU Y/AU
L1 21 S E3,E7
E MU YONG/AU
L2 22 S E5,E11
L3 2 S (US20030078371 OR US20020077280)/PN OR (WO2001-US14000 OR WO2
E ADV MED/PA,CS
L4 2 S E5,E6
E ADVAN MED/PA,CS
E ADVANC MED/PA,CS
E ADVANCED MED/PA,CS
L5 60 S E5-E9,E65-E77
L6 101 S L1-L5
SEL RN
DEL SEL

FILE 'REGISTRY' ENTERED AT 09:44:08 ON 06 APR 2004

FILE 'HCAPLUS' ENTERED AT 09:44:08 ON 06 APR 2004

SET SMARTSELECT ON
L7 SEL L6 1- RN : 3410 TERMS
SET SMARTSELECT OFF

FILE 'REGISTRY' ENTERED AT 09:44:12 ON 06 APR 2004

L8 3410 S L7
L9 505 S L8 AND VANCOMY?
L10 306 S L8 AND S/ELS
L11 113 S L9 AND L10
E 23290/RID
L12 3379 S E3
L13 505 S L8 AND L12
L14 565 S L12 AND S/ELS
L15 555 S L14 AND OC5/ES
L16 10 S L14 NOT L15
L17 3476 S L12 OR ?VANCOMYCIN?/CNS
L18 97 S L17 NOT L12
L19 96 S L18 NOT CCS/CI
L20 40 S L19 NOT SQL/FA
L21 36 S L20 NOT ?TRANSFERASE?/CNS
L22 61 S L18 NOT L21

L23 3415 S L17 NOT L22
L24 565 S L23 AND S/ELS
L25 STR
L26 36 S L25
L27 STR L25
L28 50 S L27
L29 9849 S L27 FUL
SAV TEMP L29 KAM847/A
L30 0 S L29 AND L23
L31 0 S L29 AND ?VANCOMYCIN?/CNS

FILE 'HCAPLUS' ENTERED AT 09:52:27 ON 06 APR 2004

L32 5597 S L23
L33 6924 S ?VANCOMYCIN?
L34 7296 S L32,L33
L35 12614 S L29
L36 7 S L34 AND L35
L37 0 S L6 AND L36
SEL HIT RN L36

FILE 'REGISTRY' ENTERED AT 09:54:58 ON 06 APR 2004

L38 12 S E1-E12
L39 2 S L38 AND L23
L40 10 S L38 AND L29
L41 STR L27
L42 90 S L41 FUL SUB=L29
SAV L42 KAM847A/A
L43 32 S L42 AND (C18H34O2S OR C7H12O2S OR C8H14O2S OR C13H16O2S OR C7
L44 58 S L42 NOT L43
L45 2 S L44 AND (C18H34O2S OR C7H12O2S)
L46 34 S L43,L45
SAV L46 KAM847B/A

FILE 'HCAPLUS' ENTERED AT 10:46:30 ON 06 APR 2004

L47 37 S L46
L48 0 S L47 AND L6
L49 0 S L47 AND L34
L50 26 S L46 (L) RACT+NT/RL

FILE 'REGISTRY' ENTERED AT 10:48:05 ON 06 APR 2004

L51 STR L41
L52 46 S L51 SAM SUB=L29
L53 826 S L51 FUL SUB=L29
SAV TEMP L53 KAM847C/A
L54 STR L51
L55 25 S L54 CSS SAM SUB=L29
L56 509 S L54 CSS FUL SUB=L29
SAV TEMP L56 KAM847D/A

FILE 'HCAPLUS' ENTERED AT 10:52:48 ON 06 APR 2004

L57 170 S L56
L58 0 S L57 AND L50
L59 0 S L57 AND L47

FILE 'REGISTRY' ENTERED AT 10:53:29 ON 06 APR 2004

=> => fil reg

FILE 'REGISTRY' ENTERED AT 11:00:45 ON 06 APR 2004

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provided by InfoChem.

STRUCTURE FILE UPDATES: 4 APR 2004 HIGHEST RN 671180-42-0
DICTIONARY FILE UPDATES: 4 APR 2004 HIGHEST RN 671180-42-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que l64

L12 3379 SEA FILE=REGISTRY ABB=ON PLU=ON 23290/RID
L17 3476 SEA FILE=REGISTRY ABB=ON PLU=ON L12 OR ?VANCOMYCIN?/CNS
L18 97 SEA FILE=REGISTRY ABB=ON PLU=ON L17 NOT L12
L19 96 SEA FILE=REGISTRY ABB=ON PLU=ON L18 NOT CCS/CI
L20 40 SEA FILE=REGISTRY ABB=ON PLU=ON L19 NOT SQL/FA
L21 36 SEA FILE=REGISTRY ABB=ON PLU=ON L20 NOT ?TRANSFERASE?/CNS
L22 61 SEA FILE=REGISTRY ABB=ON PLU=ON L18 NOT L21
L23 3415 SEA FILE=REGISTRY ABB=ON PLU=ON L17 NOT L22
L60 STR

6
O
||
||
2 C---S
3

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 3

STEREO ATTRIBUTES: NONE

L62 3476 SEA FILE=REGISTRY ABB=ON PLU=ON (L17 OR L23)

L64 45 SEA FILE=REGISTRY SUB=L62 SSS FUL L60

100.0% PROCESSED 45 ITERATIONS

45 ANSWERS

SEARCH TIME: 00.00.01

=> d his

(FILE 'HOME' ENTERED AT 09:40:00 ON 06 APR 2004)

SET COST OFF

FILE 'HCAPLUS' ENTERED AT 09:40:16 ON 06 APR 2004

E MU Y/AU

L1 21 S E3,E7

E MU YONG/AU

L2 22 S E5,E11

L3 2 S (US20030078371 OR US20020077280)/PN OR (WO2001-US14000 OR WO2
E ADV MED/PA,CS

L4 2 S E5,E6
E ADVAN MED/PA,CS
E ADVANC MED/PA,CS
E ADVANCED MED/PA,CS
L5 60 S E5-E9,E65-E77
L6 101 S L1-L5
SEL RN
DEL SEL

FILE 'REGISTRY' ENTERED AT 09:44:08 ON 06 APR 2004

FILE 'HCAPLUS' ENTERED AT 09:44:08 ON 06 APR 2004

SET SMARTSELECT ON
L7 SEL L6 1- RN : 3410 TERMS
SET SMARTSELECT OFF

FILE 'REGISTRY' ENTERED AT 09:44:12 ON 06 APR 2004

L8 3410 S L7
L9 505 S L8 AND VANCOMY?
L10 306 S L8 AND S/ELS
L11 113 S L9 AND L10
E 23290/RID
L12 3379 S E3
L13 505 S L8 AND L12
L14 565 S L12 AND S/ELS
L15 555 S L14 AND OC5/ES
L16 10 S L14 NOT L15
L17 3476 S L12 OR ?VANCOMYCIN?/CNS
L18 97 S L17 NOT L12
L19 96 S L18 NOT CCS/CI
L20 40 S L19 NOT SQL/FA
L21 36 S L20 NOT ?TRANSFERASE?/CNS
L22 61 S L18 NOT L21
L23 3415 S L17 NOT L22
L24 565 S L23 AND S/ELS
L25 STR
L26 36 S L25
L27 STR L25
L28 50 S L27
L29 9849 S L27 FUL
SAV TEMP L29 KAM847/A
L30 0 S L29 AND L23
L31 0 S L29 AND ?VANCOMYCIN?/CNS

FILE 'HCAPLUS' ENTERED AT 09:52:27 ON 06 APR 2004

L32 5597 S L23
L33 6924 S ?VANCOMYCIN?
L34 7296 S L32,L33
L35 12614 S L29
L36 7 S L34 AND L35
L37 0 S L6 AND L36
SEL HIT RN L36

FILE 'REGISTRY' ENTERED AT 09:54:58 ON 06 APR 2004

L38 12 S E1-E12
L39 2 S L38 AND L23
L40 10 S L38 AND L29
L41 STR L27
L42 90 S L41 FUL SUB=L29
SAV L42 KAM847A/A
L43 32 S L42 AND (C18H34O2S OR C7H12O2S OR C8H14O2S OR C13H16O2S OR C7
L44 58 S L42 NOT L43
L45 2 S L44 AND (C18H34O2S OR C7H12O2S)

L46 34 S L43,L45
SAV L46 KAM847B/A

FILE 'HCAPLUS' ENTERED AT 10:46:30 ON 06 APR 2004

L47 37 S L46
L48 0 S L47 AND L6
L49 0 S L47 AND L34
L50 26 S L46 (L) RACT+NT/RL

FILE 'REGISTRY' ENTERED AT 10:48:05 ON 06 APR 2004

L51 STR L41
L52 46 S L51 SAM SUB=L29
L53 826 S L51 FUL SUB=L29
SAV TEMP L53 KAM847C/A
L54 STR L51
L55 25 S L54 CSS SAM SUB=L29
L56 509 S L54 CSS FUL SUB=L29
SAV TEMP L56 KAM847D/A

FILE 'HCAPLUS' ENTERED AT 10:52:48 ON 06 APR 2004

L57 170 S L56
L58 0 S L57 AND L50
L59 0 S L57 AND L47

FILE 'REGISTRY' ENTERED AT 10:53:29 ON 06 APR 2004

L60 STR L27
L61 0 S L60 SAM SUB=L24
L62 3476 S L17,L23
L63 0 S L60 SAM SUB=L62
L64 45 S L60 FUL SUB=L62
SAV L64 KAM847E/A

FILE 'HCAPLUS' ENTERED AT 11:00:25 ON 06 APR 2004

L65 3 S L64

FILE 'REGISTRY' ENTERED AT 11:00:45 ON 06 APR 2004

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 11:00:56 ON 06 APR 2004

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FILE COVERS 1907 - 6 Apr 2004 VOL 140 ISS 15
FILE LAST UPDATED: 5 Apr 2004 (20040405/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l65 all hitstr tot

L65 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:689112 HCAPLUS
DN 136:70060
ED Entered STN: 20 Sep 2001
TI Synthesis and biological evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria: target-accelerated combinatorial synthesis
AU Nicolaou, K. C.; Hughes, Robert; Cho, Suk Young; Winssinger, Nicolas; Labischinski, Harald; Endermann, Rainer
CS Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SO Chemistry--A European Journal (2001), 7(17), 3824-3843
CODEN: CEUJED; ISSN: 0947-6539
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 33
AB Based on the notion that dimerization and/or variation of amino acid 1 of vancomycin could potentially enhance biol. activity, a series of synthetic and chemical biol. studies were undertaken in order to discover potent antibacterial agents. We describe two ligation methods (disulfide formation and olefin metathesis) for dimerizing vancomycin derivs. and applications of target-accelerated combinatorial synthesis (e.g., combinatorial synthesis in the presence of vancomycin's target Ac2-L-Lys-D-Ala-D-Ala) to generate libraries of vancomycin dimers. Screening of these compound libraries led to the identification of a number of highly potent antibiotics effective against vancomycin-susceptible, vancomycin-intermediate resistant and, most significantly, vancomycin-resistant bacteria.
ST target accelerated combinatorial synthesis vancomycin dimer library; ligation disulfide formation olefin metathesis vancomycin dimer synthesis; vancomycin dimer prepn antibacterial
IT Peptides, preparation
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation)
(oligopeptides; synthesis and biol. evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria, including target-accelerated combinatorial synthesis)
IT Antibacterial agents
Peptide library
(synthesis and biol. evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria, including target-accelerated combinatorial synthesis)
IT Combinatorial chemistry
(target-accelerated; synthesis and biol. evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria, including target-accelerated combinatorial synthesis)
IT 321361-75-5P 383185-24-8P 383185-26-0P 383185-28-2P 383185-30-6P
RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)
(synthesis and biol. evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria, including target-accelerated combinatorial synthesis)
IT 1404-90-6DP, Vancomycin, dimeric derivs. 321361-73-3P 321361-77-7P 321361-81-3P 383185-34-0P 383185-37-3P 383383-25-3P
RL: CPN (Combinatorial preparation); PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation)
(synthesis and biol. evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria, including target-accelerated combinatorial synthesis)

IT 1119-94-4, Dodecyltrimethylammonium bromide 19993-26-1 105149-26-6
RL: CRG (Combinatorial reagent); RGT (Reagent); CMBI (Combinatorial study); RACT (Reactant or reagent)
(synthesis and biol. evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria, including target-accelerated combinatorial synthesis)

IT 383185-18-0 383185-20-4 383185-22-6
RL: CRT (Combinatorial reactant); RCT (Reactant); CMBI (Combinatorial study); RACT (Reactant or reagent)
(synthesis and biol. evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria, including target-accelerated combinatorial synthesis)

IT 321361-79-9P 321361-83-5P 321361-85-7P 321361-87-9P 321361-89-1P
321361-91-5P 321361-95-9P 383183-13-9P 383183-14-0P 383183-15-1P
383183-16-2P 383183-17-3P 383183-18-4P 383183-19-5P 383183-20-8P
383183-21-9P 383183-22-0P 383183-23-1P 383183-24-2P 383183-25-3P
383183-26-4P 383183-28-6P 383183-29-7P 383183-48-0P 383183-49-1P
383183-50-4P 383183-51-5P 383183-52-6P 383183-53-7P 383183-54-8P
383183-55-9P 383183-56-0P 383183-57-1P 383183-58-2P 383183-59-3P
383183-60-6P 383183-61-7P 383183-62-8P 383183-63-9P 383183-64-0P
383183-66-2P 383183-67-3P 383183-68-4P 383183-69-5P 383183-70-8P
383183-83-3P 383183-84-4P 383183-85-5P 383183-86-6P 383183-87-7P
383183-88-8P 383183-89-9P 383183-90-2P 383183-91-3P 383183-92-4P
383183-93-5P 383183-94-6P 383183-95-7P 383183-96-8P 383183-99-1P
383184-01-8P 383184-03-0P 383184-06-3P 383184-09-6P 383184-10-9P
383184-11-0P 383184-13-2P 383184-15-4P 383184-17-6P 383184-21-2P
383184-23-4P 383184-26-7P 383184-27-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria, including target-accelerated combinatorial synthesis)

IT 2127-03-9 321361-97-1 321361-99-3 321362-01-0 321362-03-2
321362-05-4 321362-07-6 321362-09-8 321362-11-2 321362-13-4
321362-17-8 383183-30-0 383183-31-1
383183-32-2 383183-33-3 383183-34-4
383183-35-5 383183-36-6 383183-37-7
383183-38-8 383183-39-9 383183-40-2
383183-41-3 383183-42-4 383183-43-5
383183-44-6 383183-45-7 383183-46-8
383183-71-9 383183-72-0 383183-73-1
383183-74-2 383183-75-3 383183-76-4
383183-77-5 383183-78-6 383183-79-7
383183-80-0 383183-81-1 383183-82-2
383184-29-0 383184-31-4 383184-33-6 383184-34-7 383184-36-9
383184-39-2 383184-41-6 383184-43-8 383184-45-0 383184-47-2
383184-48-3 383184-50-7 383184-53-0 383184-56-3 383184-58-5
383184-60-9 383184-62-1 383184-65-4 383184-67-6 383184-70-1
383184-72-3 383184-76-7 383184-79-0 383184-81-4 383184-85-8
383184-87-0 383184-91-6 383184-95-0 383184-97-2
383184-99-4 383185-04-4 383185-06-6
383185-07-7 383185-09-9 383185-11-3
383185-12-4 383185-32-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis and biol. evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria, including target-accelerated combinatorial synthesis)

IT 383183-27-5P 383183-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and biol. evaluation of vancomycin dimers with potent activity against vancomycin-resistant bacteria, including target-accelerated combinatorial synthesis)

RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Adamczyk, M; Bioorg Med Chem Lett 1999, V9, P2437 HCAPLUS
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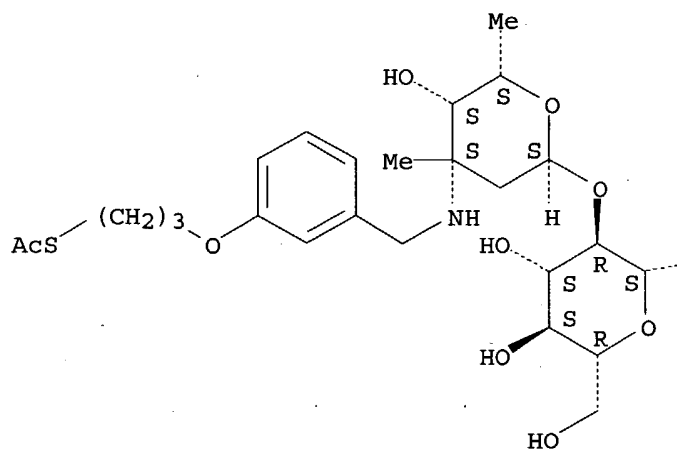
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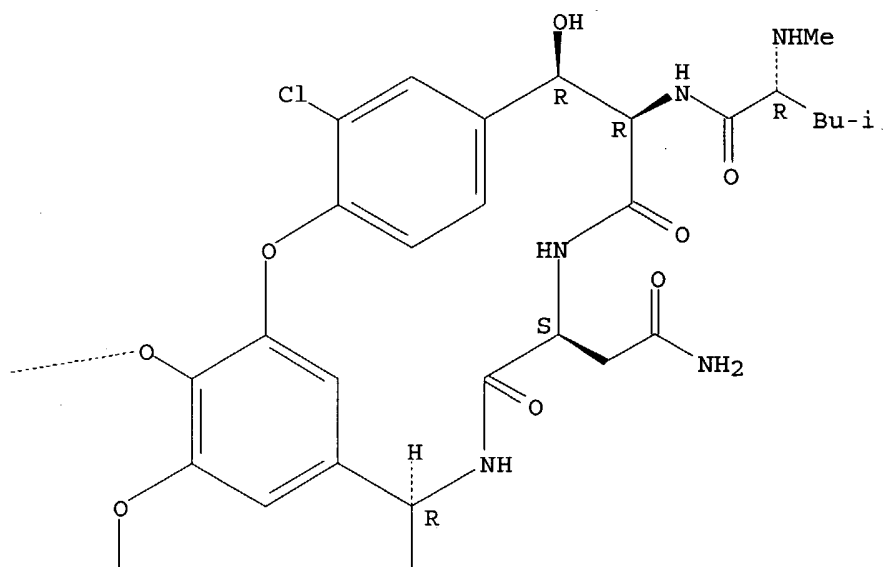
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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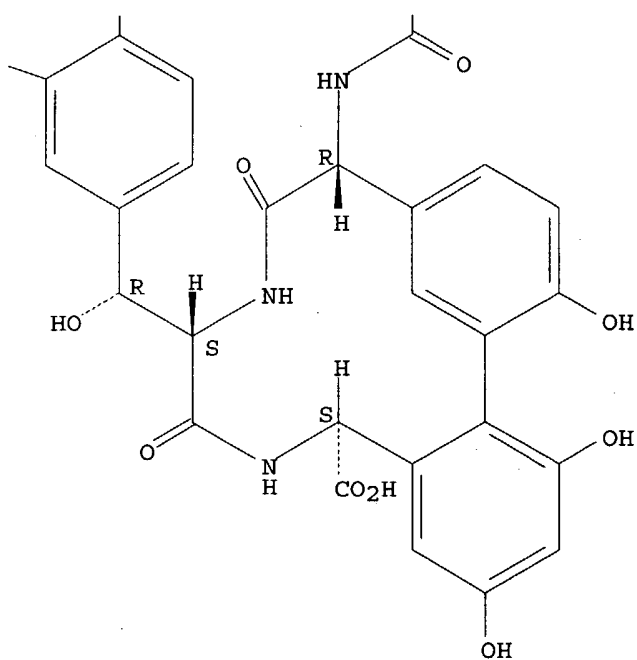
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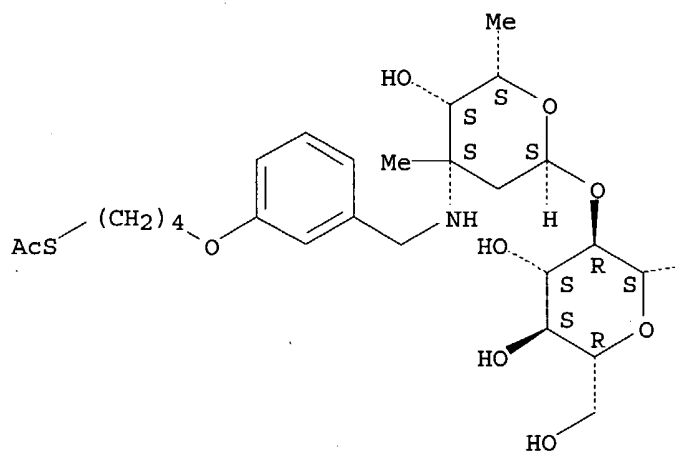
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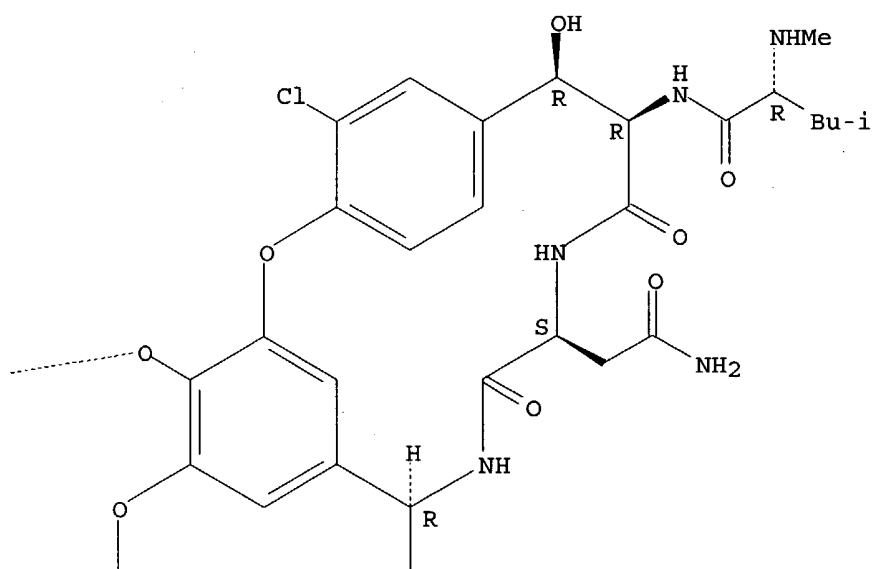


RN	569183	38	0	NCM BBS
CN	Vancomycin,	N3''-	[3-[4-(acetylthio)butoxy]phenyl]methyl]-	(9CI) (CA
	INDEX NAME)			

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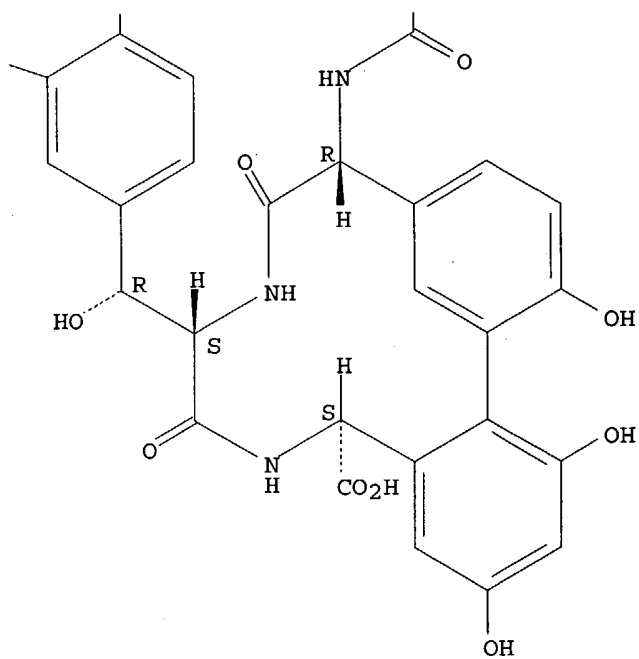
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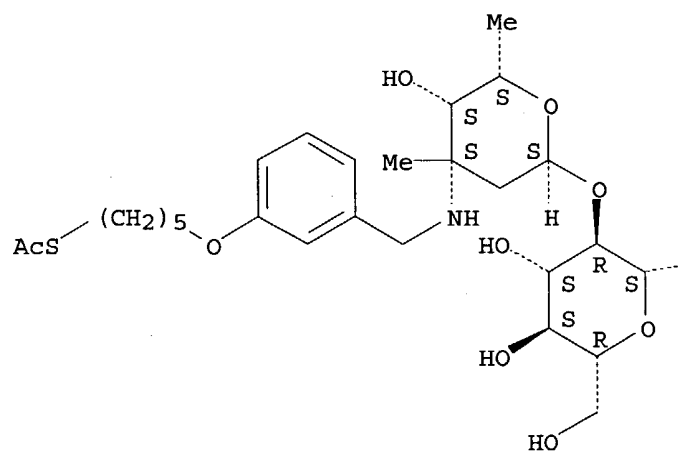


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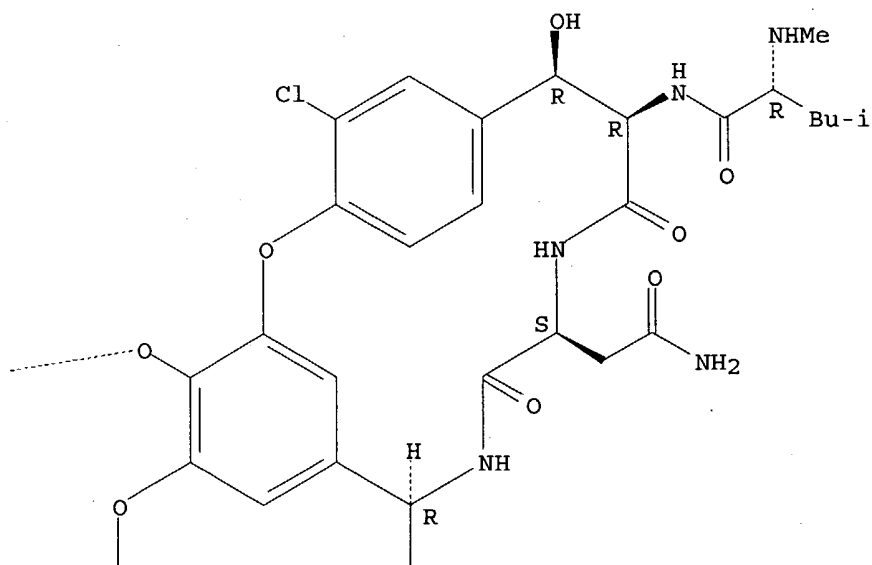
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Absolute stereochemistry.

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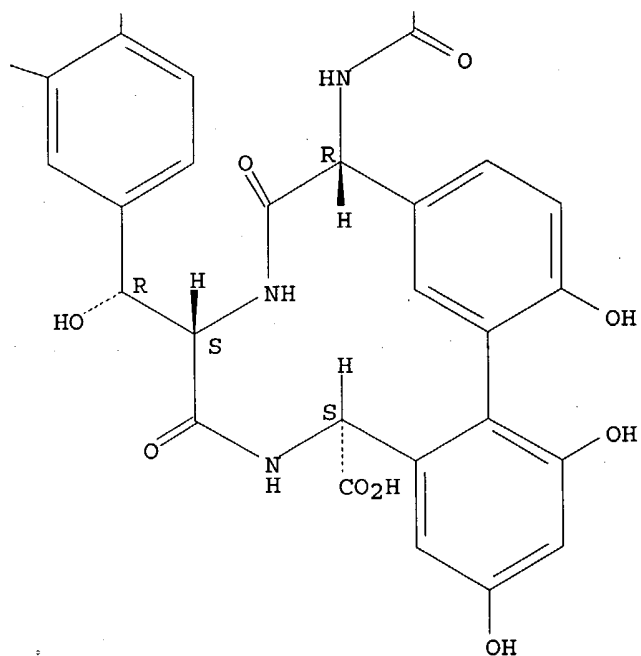
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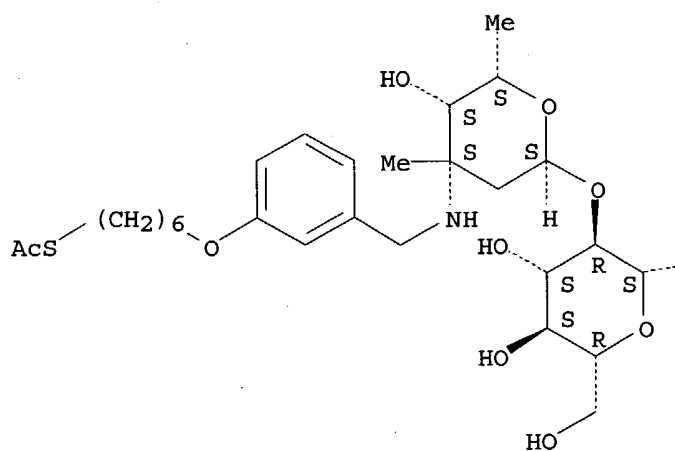


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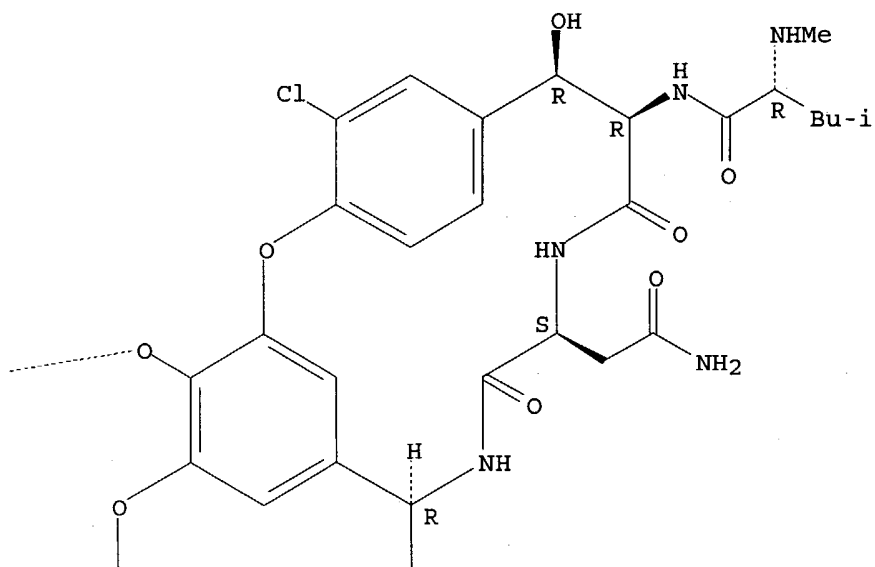
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INDEX NAME)

Absolute stereochemistry.

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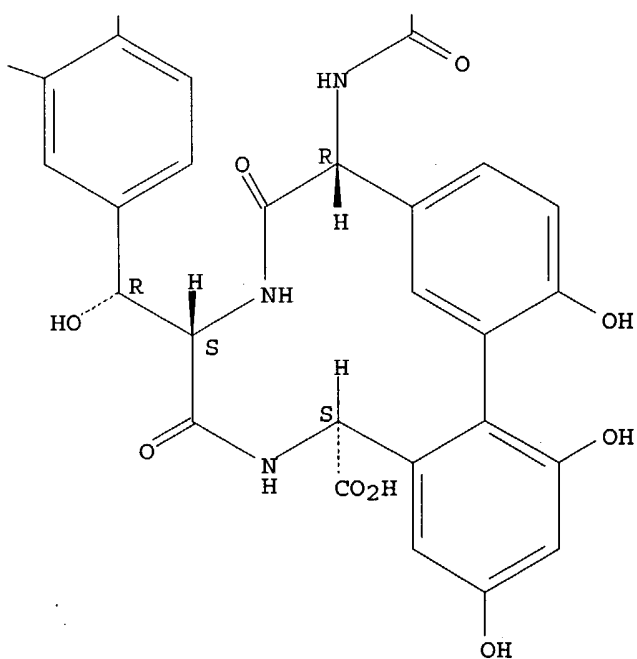
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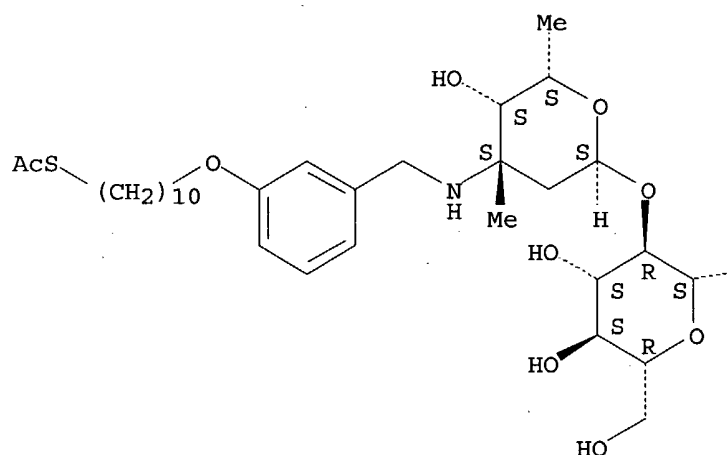


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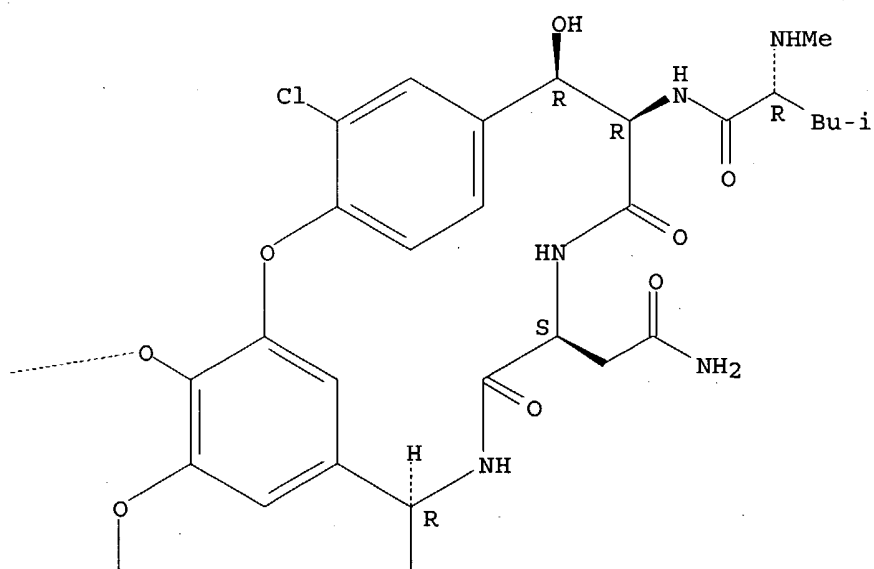
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Absolute stereochemistry.

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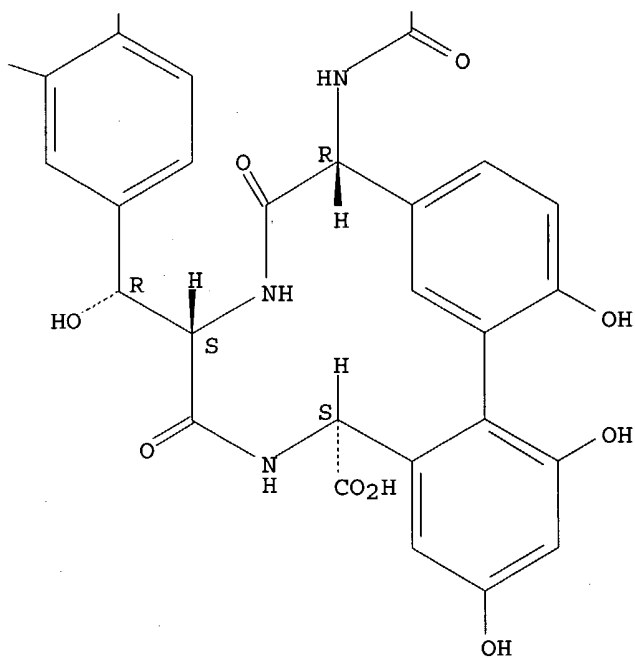
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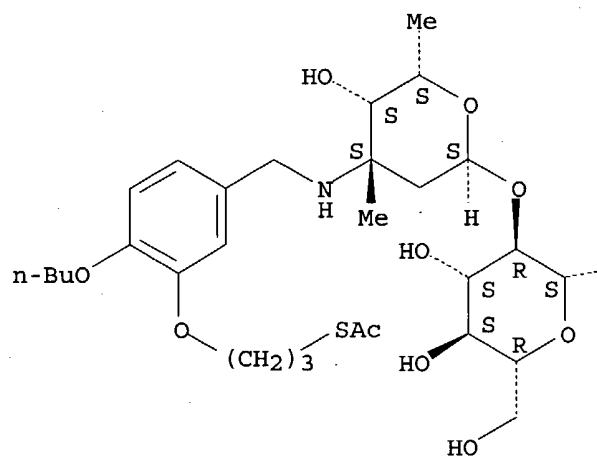


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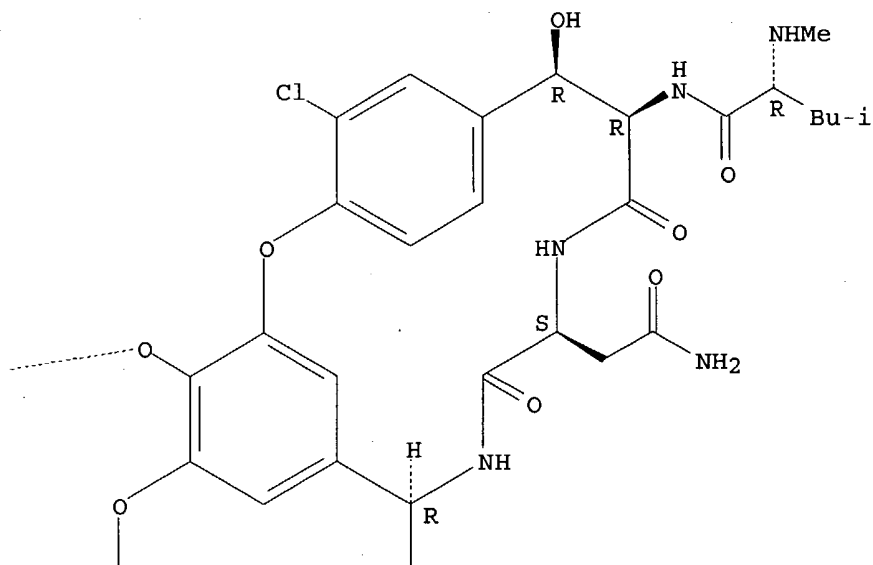
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(CA INDEX NAME)

Absolute stereochemistry.

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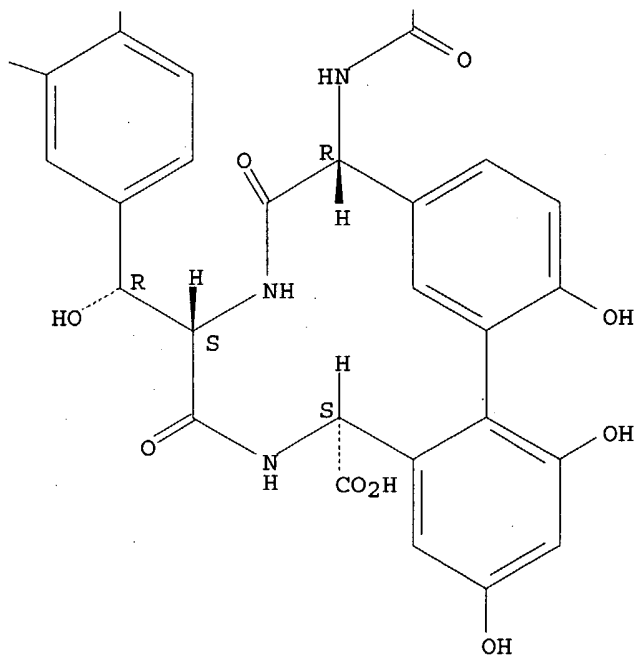
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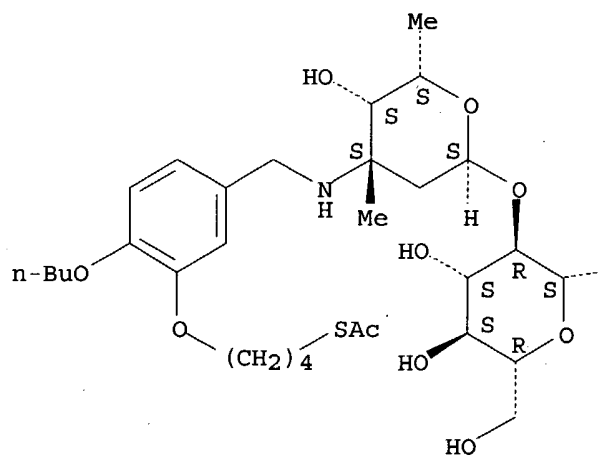


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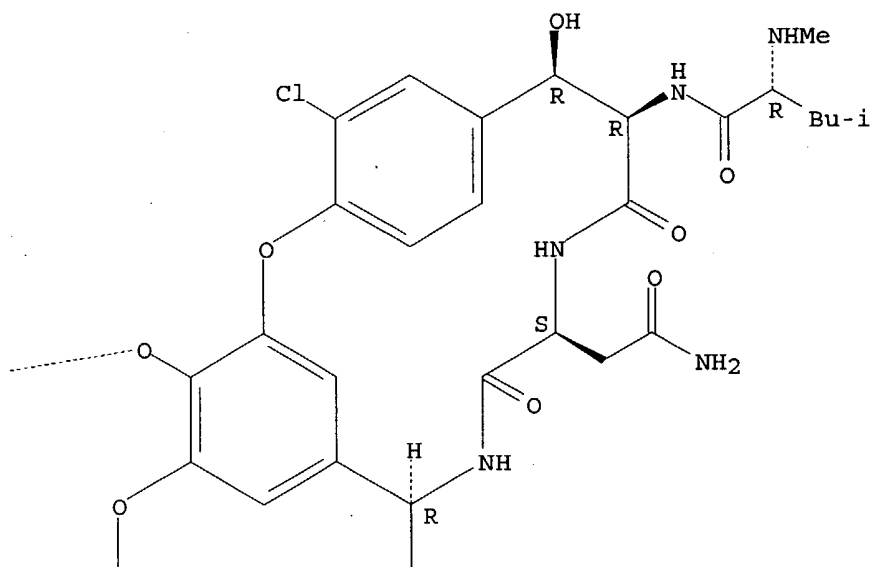
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(CA INDEX NAME)

Absolute stereochemistry.

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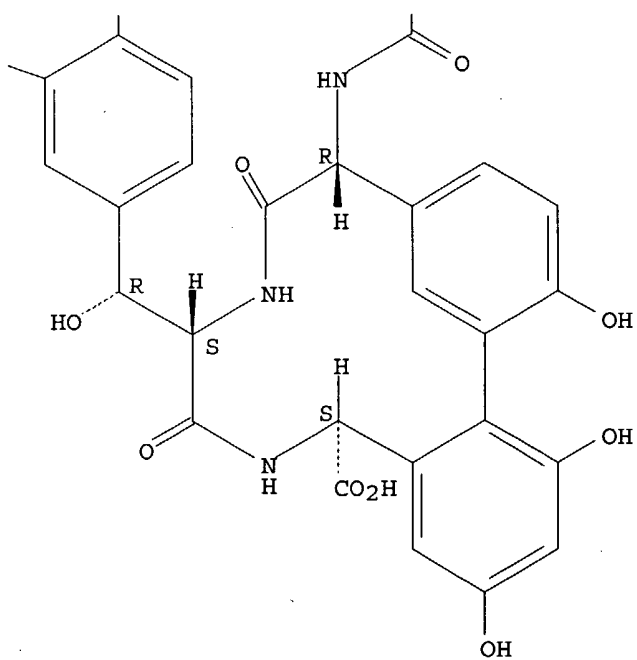
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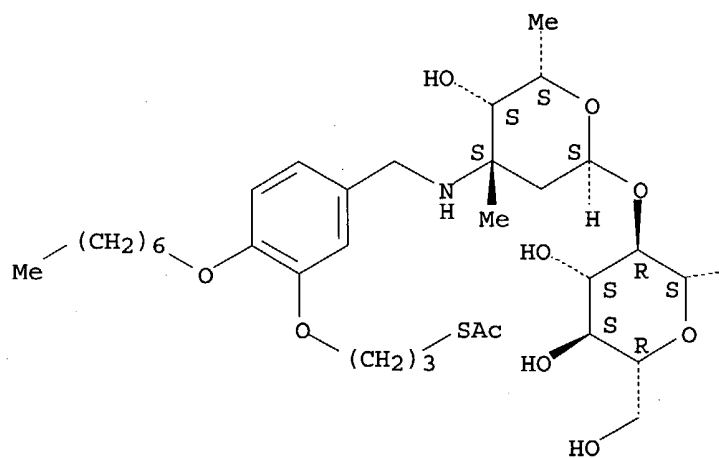


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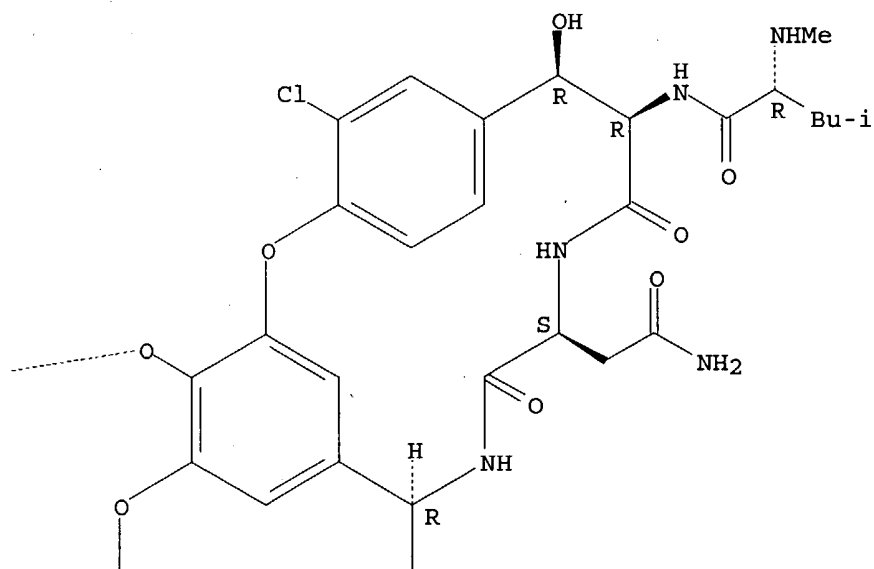
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]-4-(heptyloxy)phenyl]methyl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

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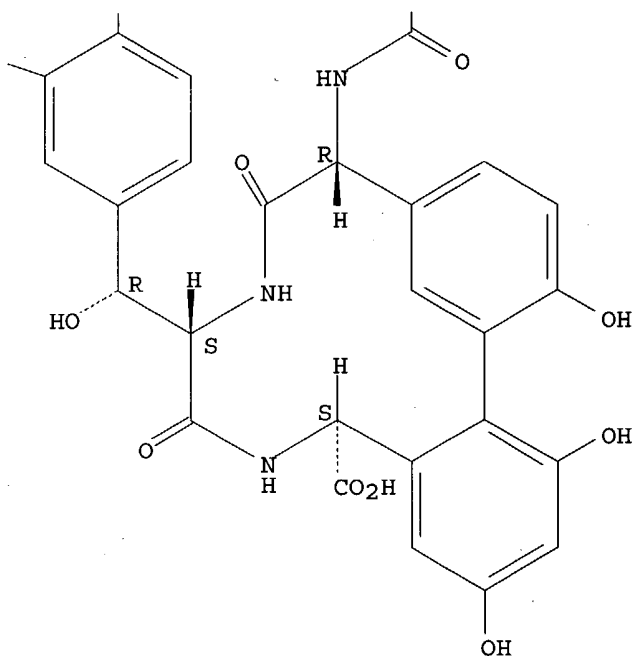
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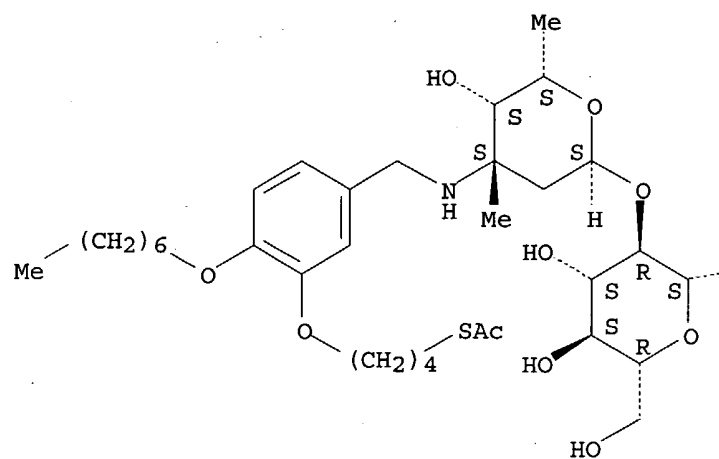


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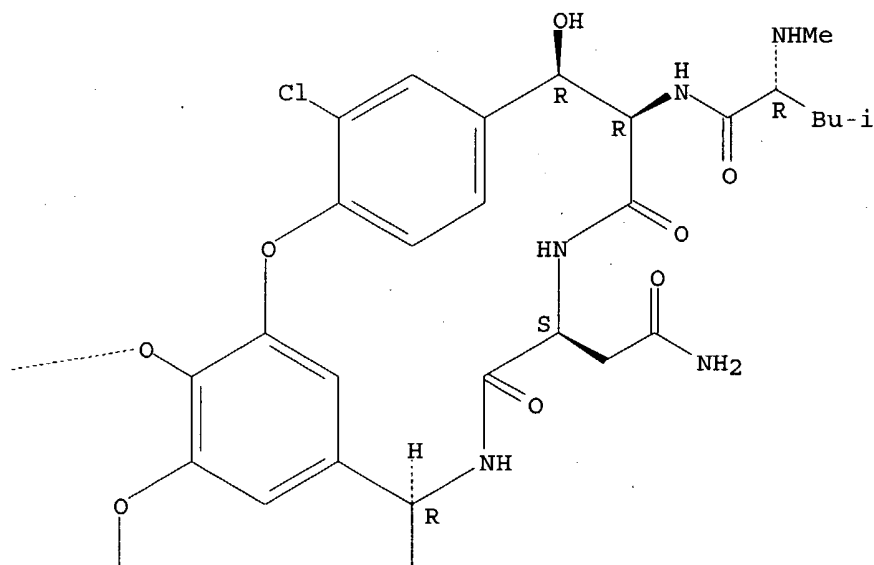
CN Vancomycin, N3'''-[3-[4-(acetylthio)butoxy]-4-(heptyloxy)phenyl]methyl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

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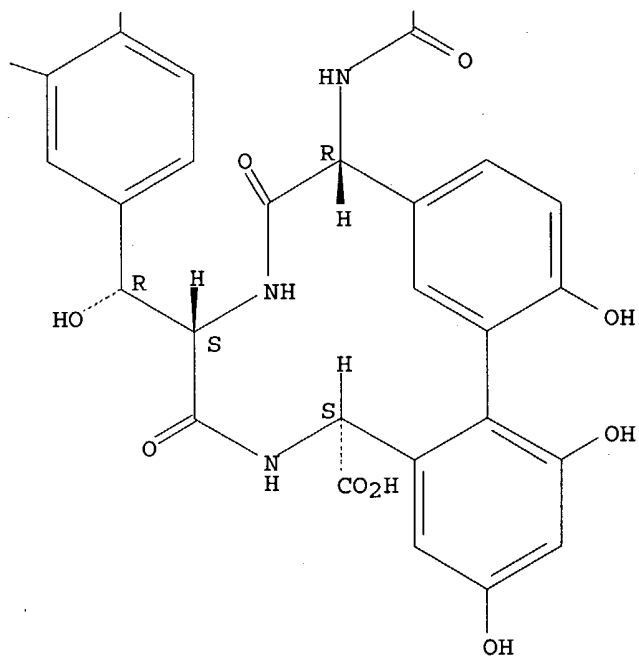
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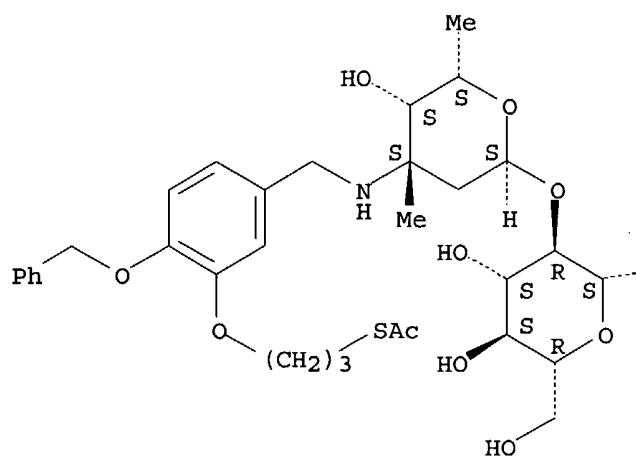


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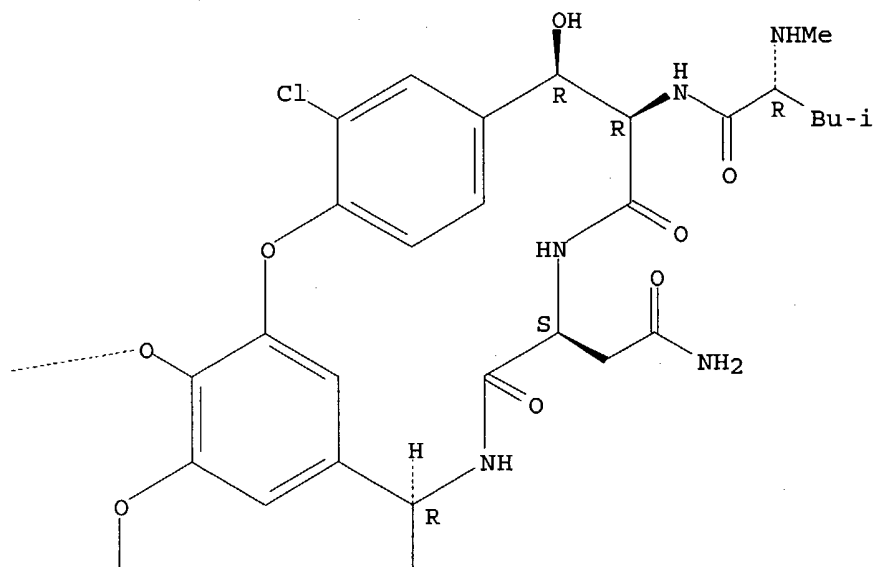
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]-4-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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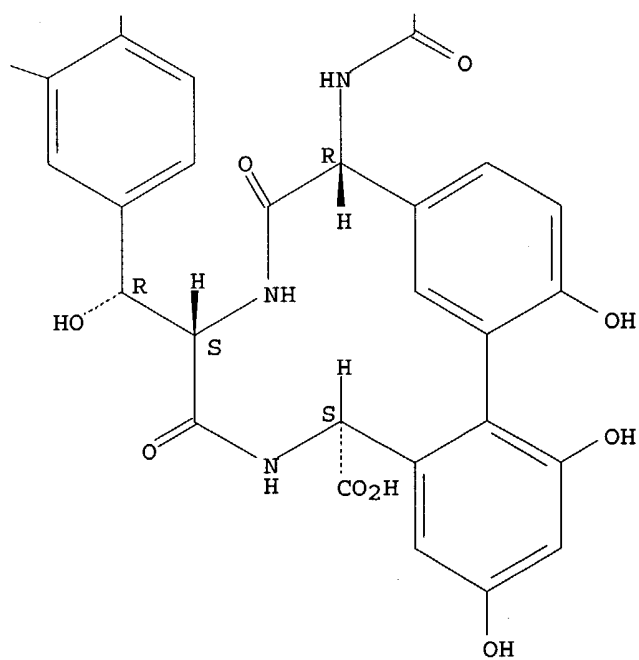
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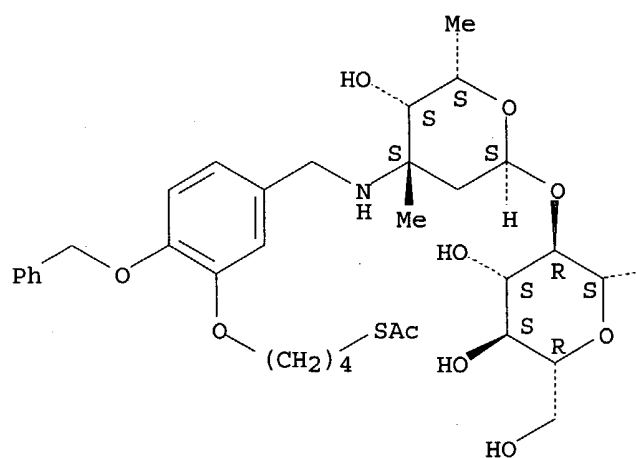


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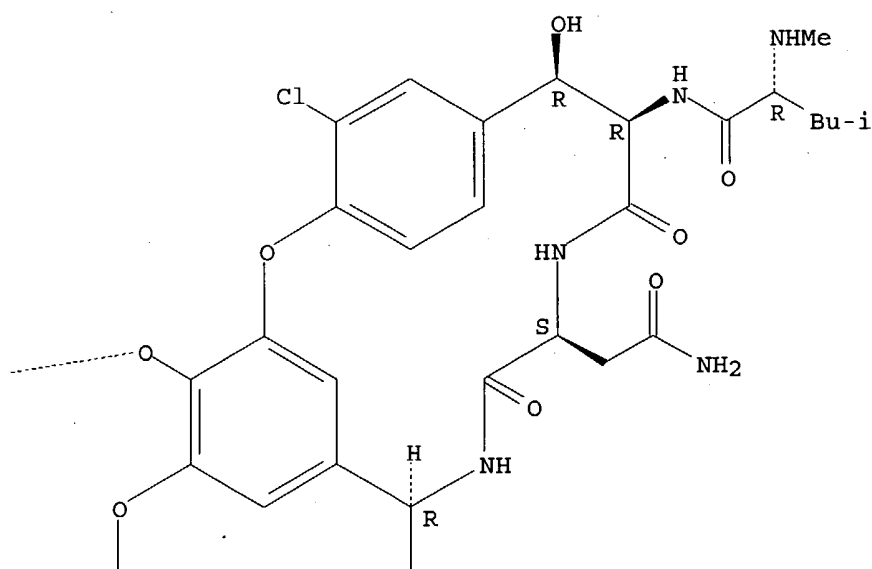
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Absolute stereochemistry.

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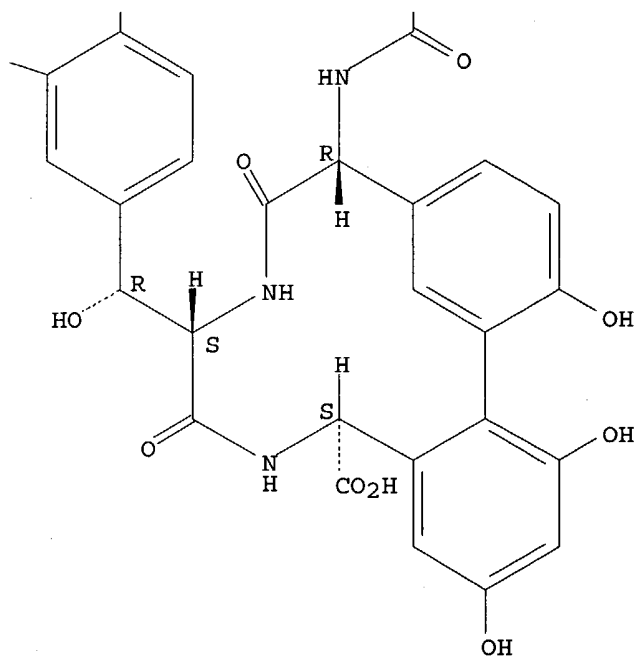
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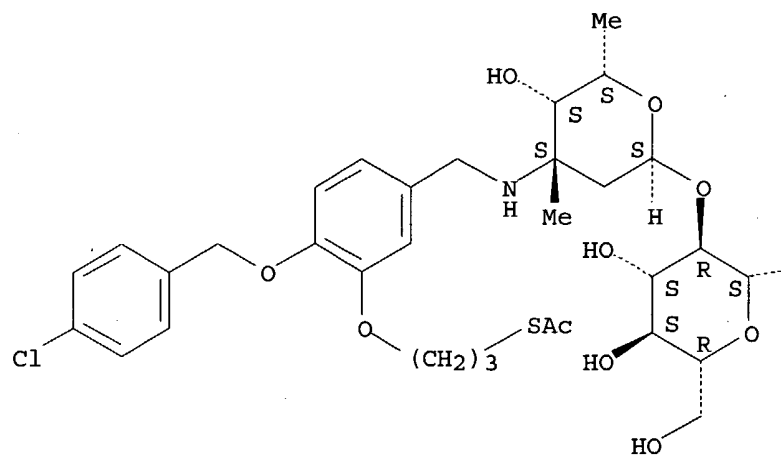


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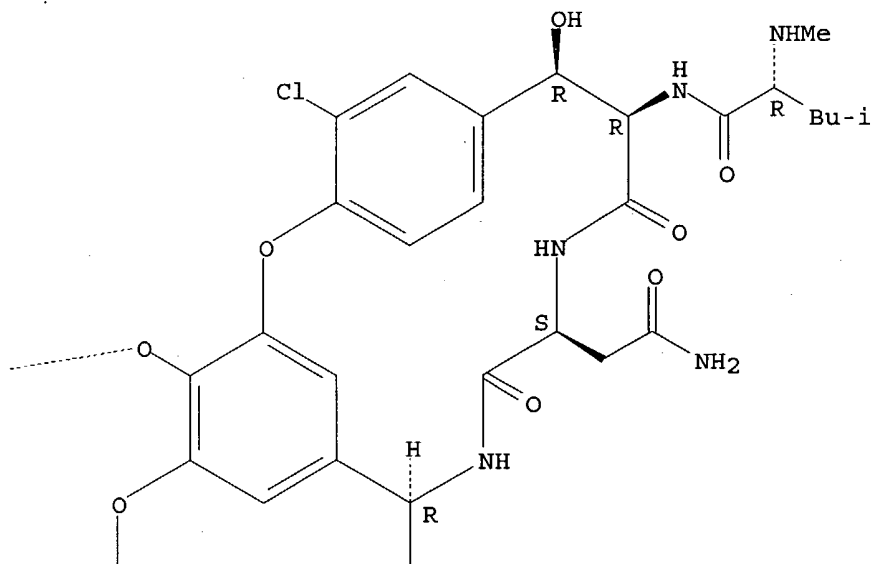
CN Vancomycin, N3'''-[3-[3-(acetylthio)propoxy]-4-[(4-chlorophenyl)methoxy]phenyl)methyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

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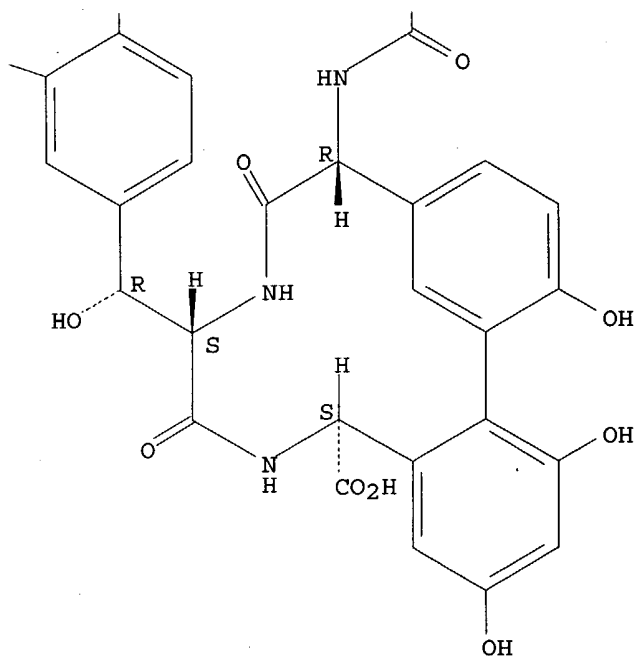
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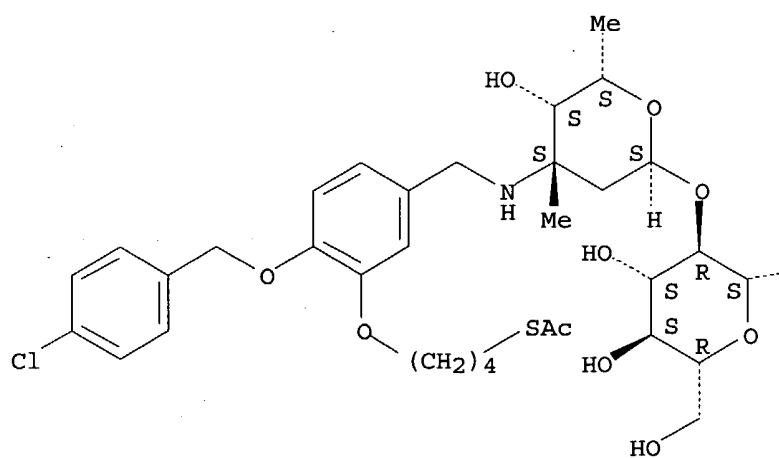


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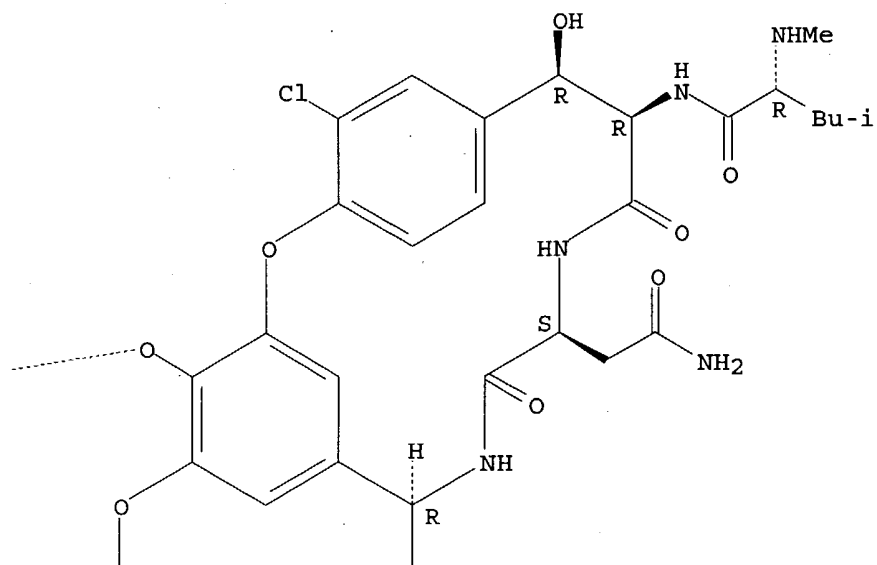
CN Vancomycin, N3''-[[3-[4-(acetylthio)butoxy]-4-[(4-chlorophenyl)methoxy]phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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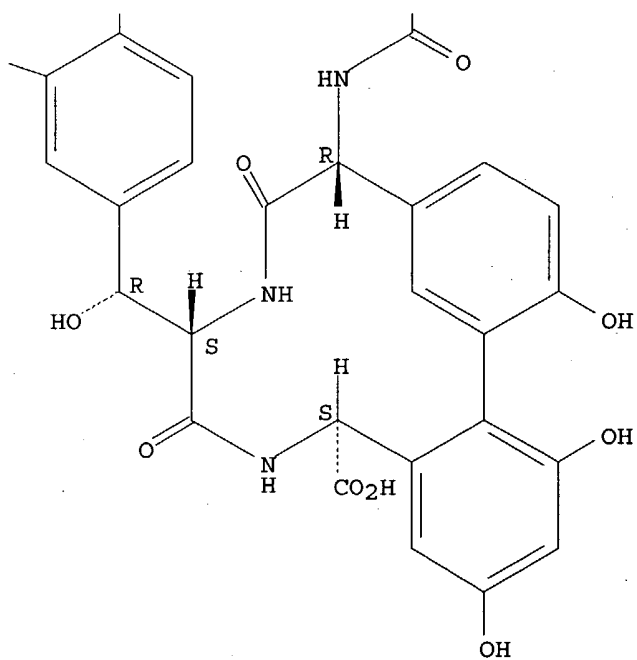
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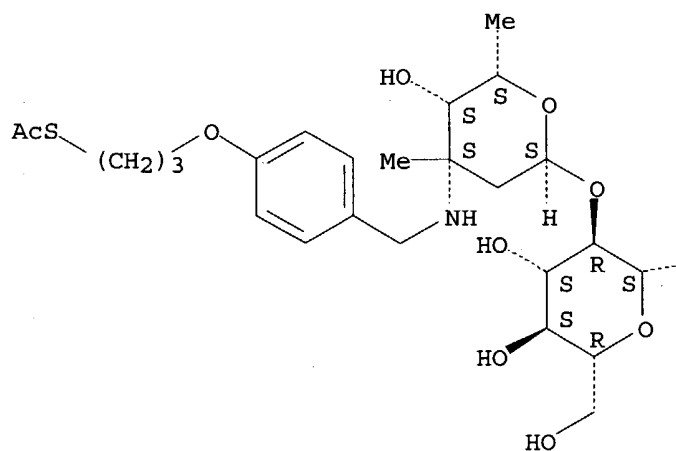


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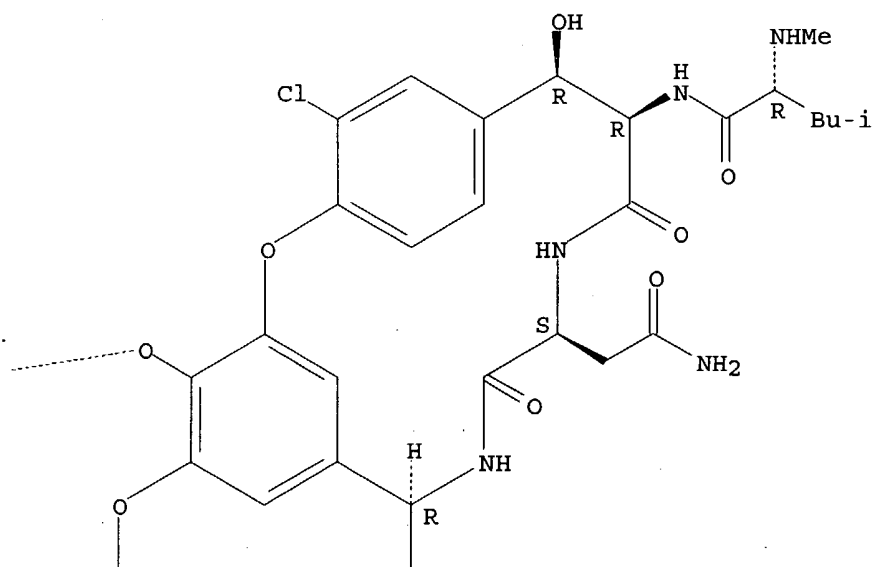
CN Vancomycin, N3'''-[[4-[3-(acetylthio)propoxy]phenyl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

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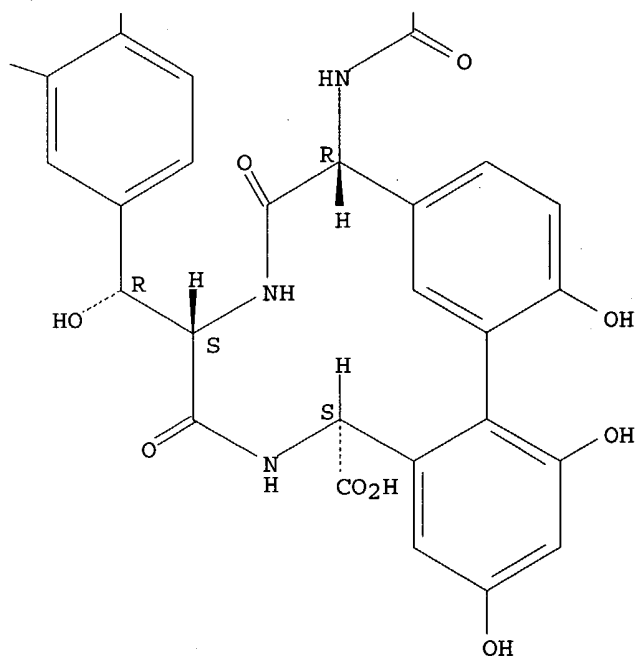
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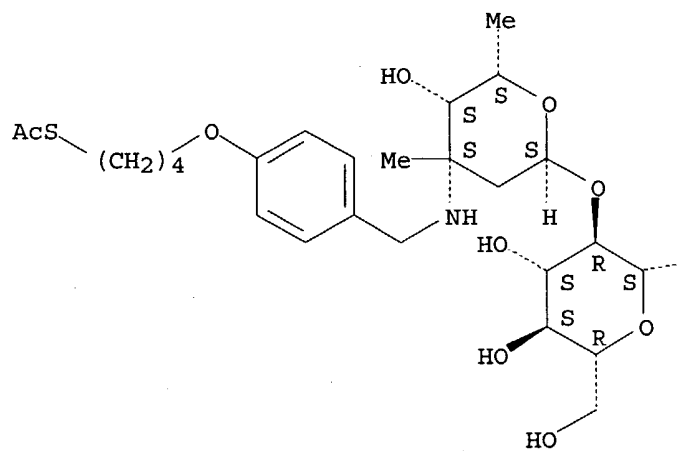


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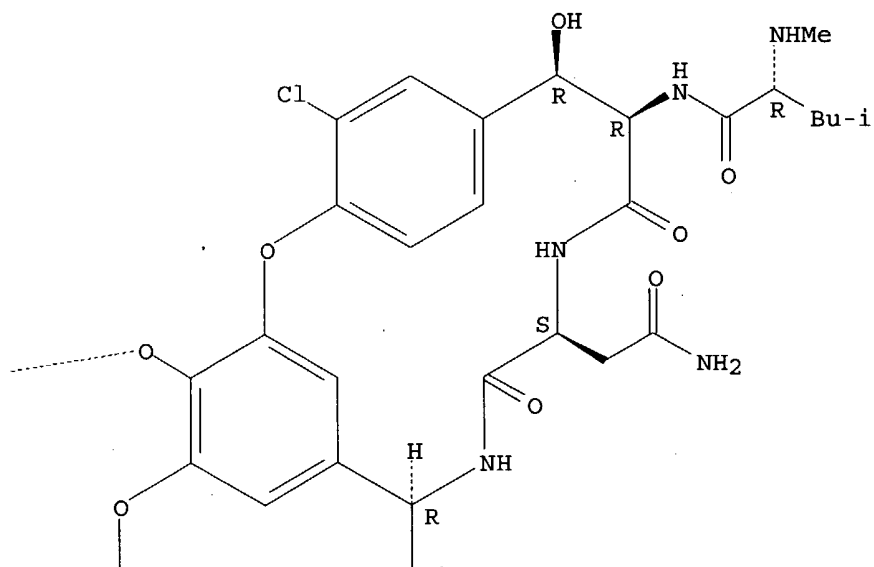
CN Vancomycin, N3'''-[[4-[4-(acetylthio)butoxy]phenyl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

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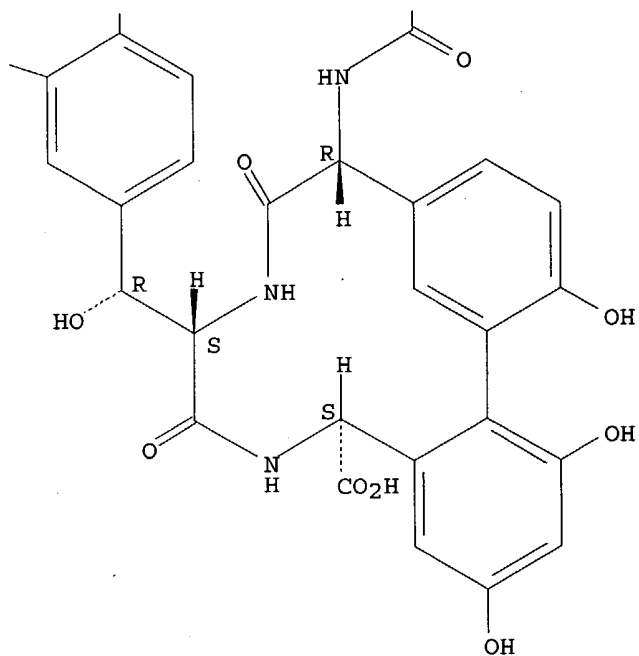
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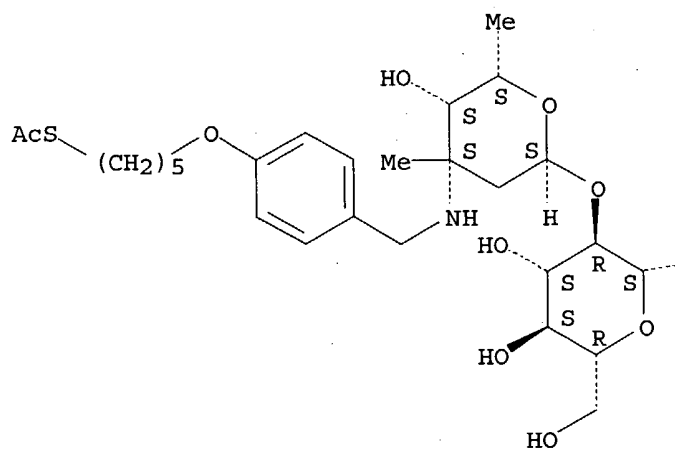


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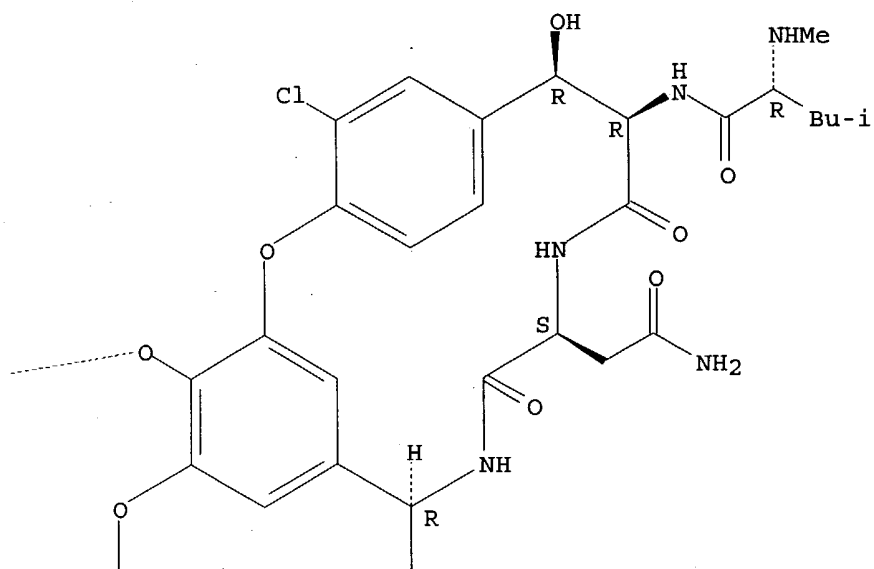
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INDEX NAME)

Absolute stereochemistry.

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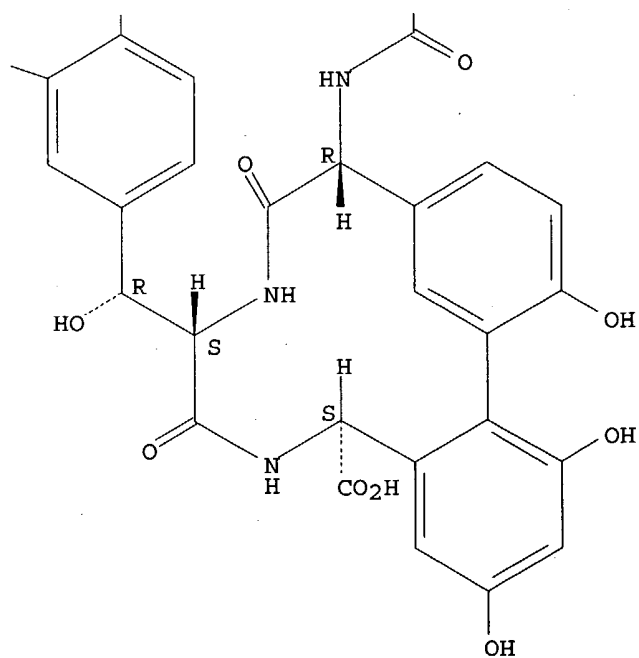
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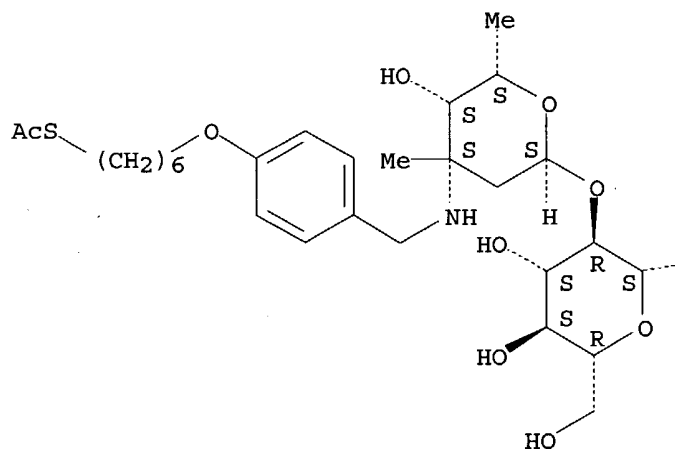


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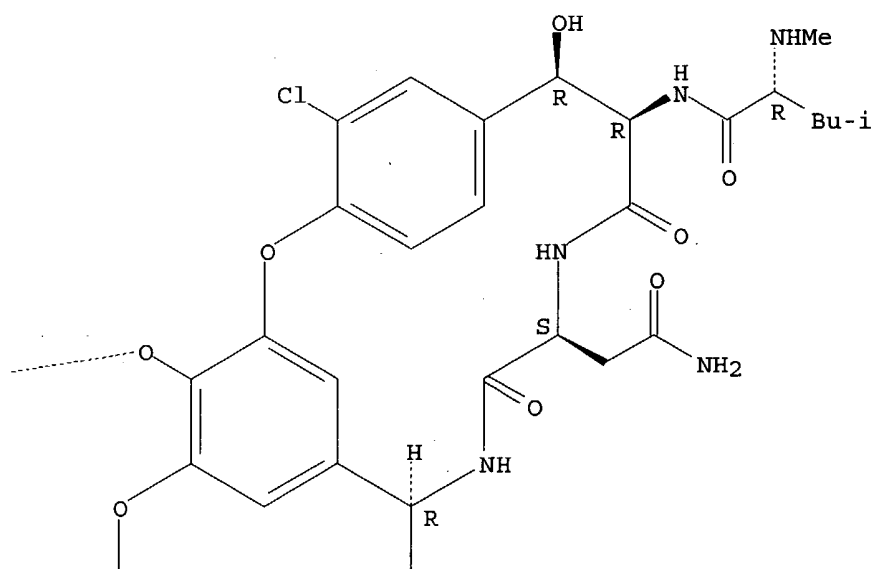
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INDEX NAME)

Absolute stereochemistry.

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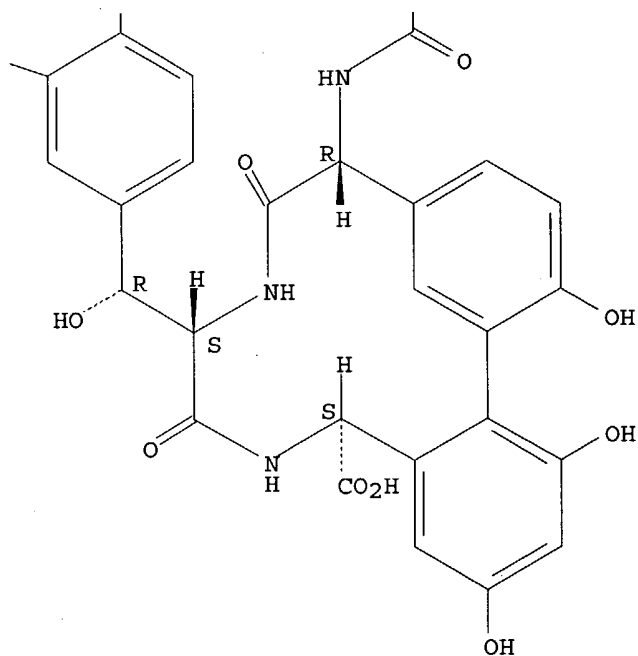
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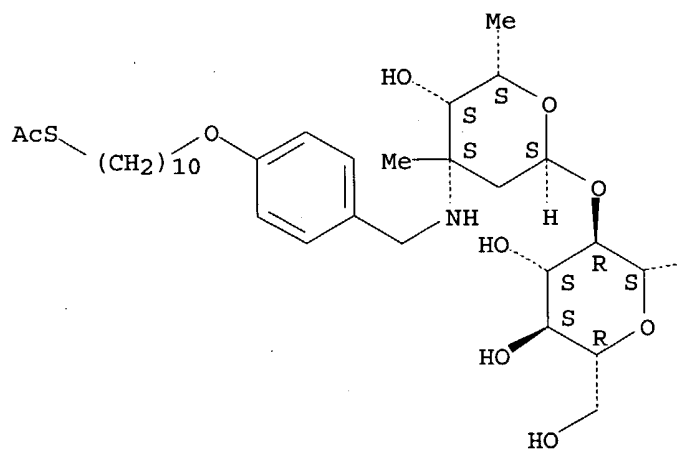


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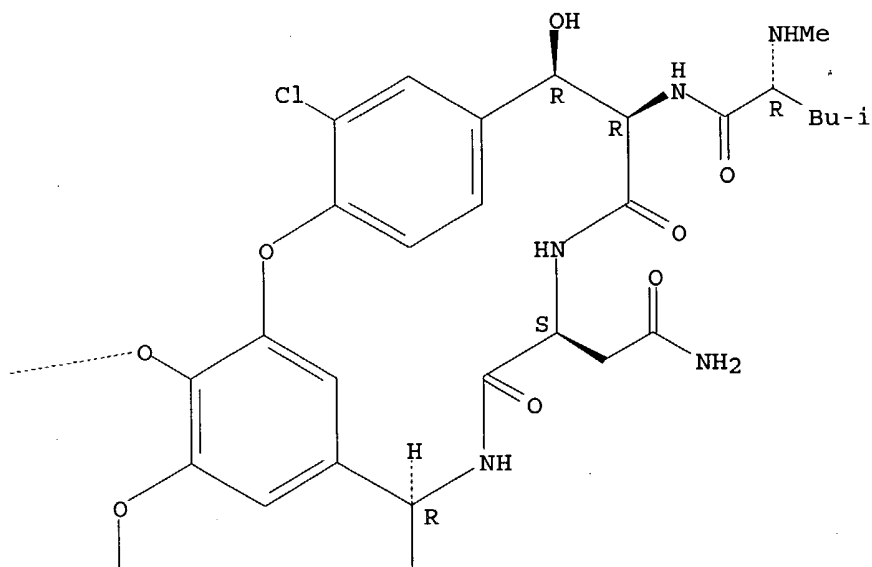
CN Vancomycin, N3'''-[[4-[[10-(acetylthio)decyl]oxy]phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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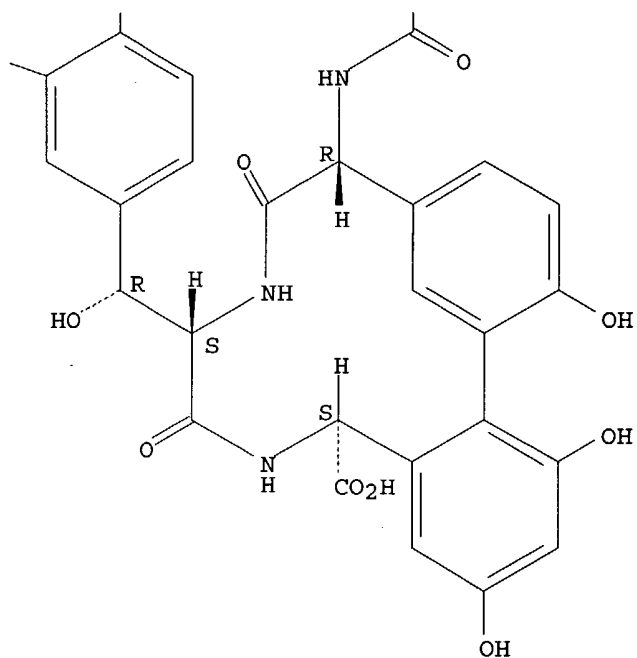
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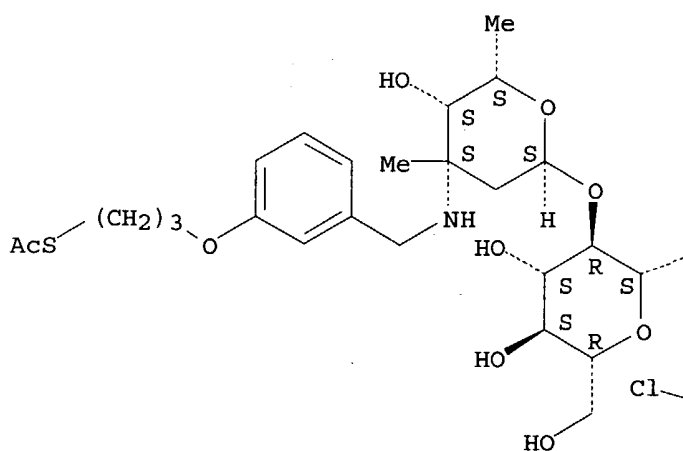


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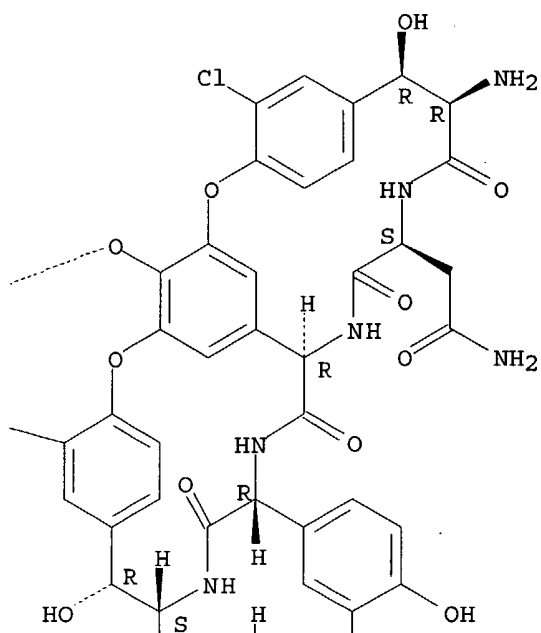
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-28-
 [[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-
 (methylamino)-1-oxopentyl]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

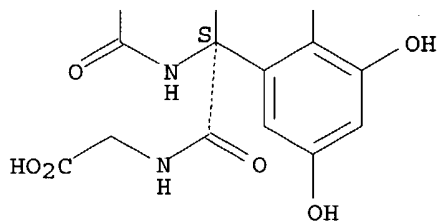
PAGE 1-A



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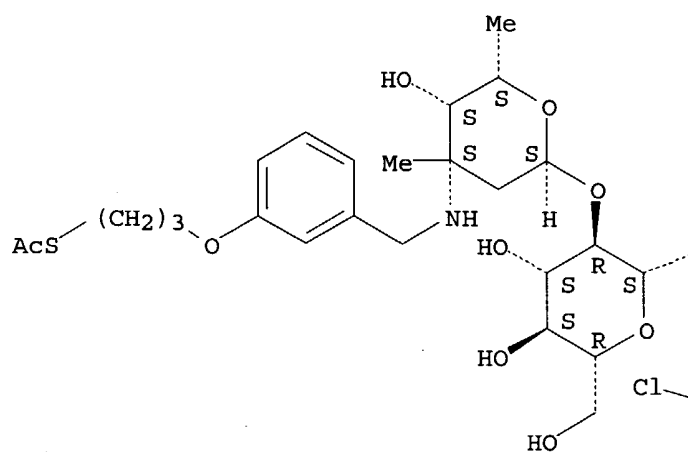


RN 383183-72-0 HCAPLUS

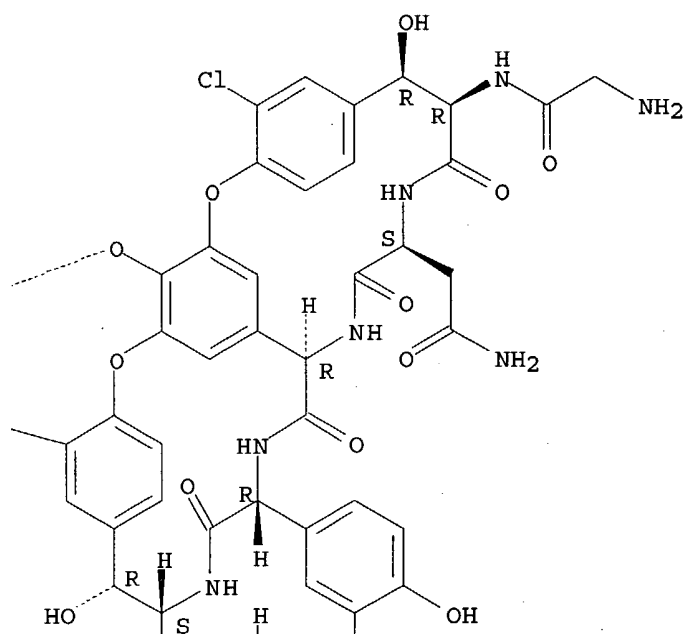
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-(aminoacetyl)-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

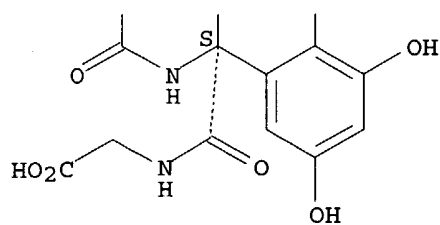
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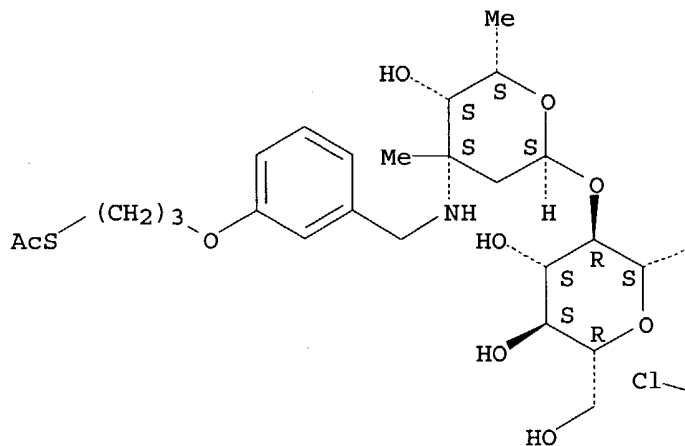


RN 383183-73-1 HCAPLUS

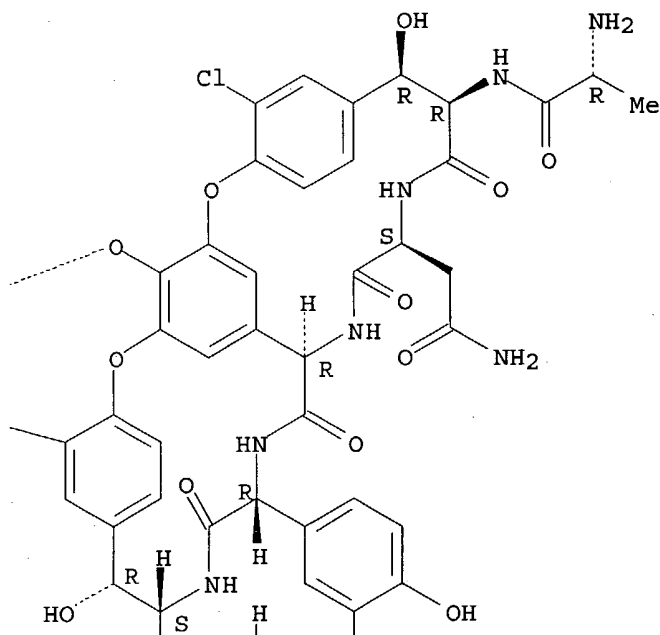
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2R)-2-amino-1-oxopropyl]-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

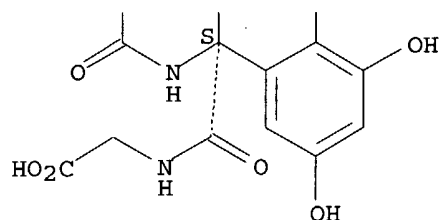
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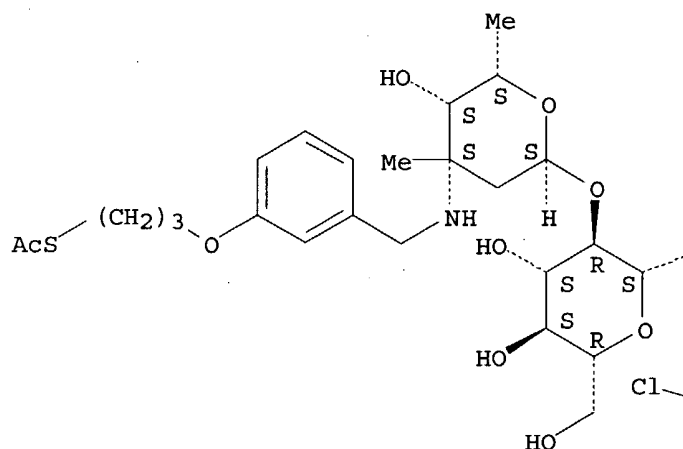


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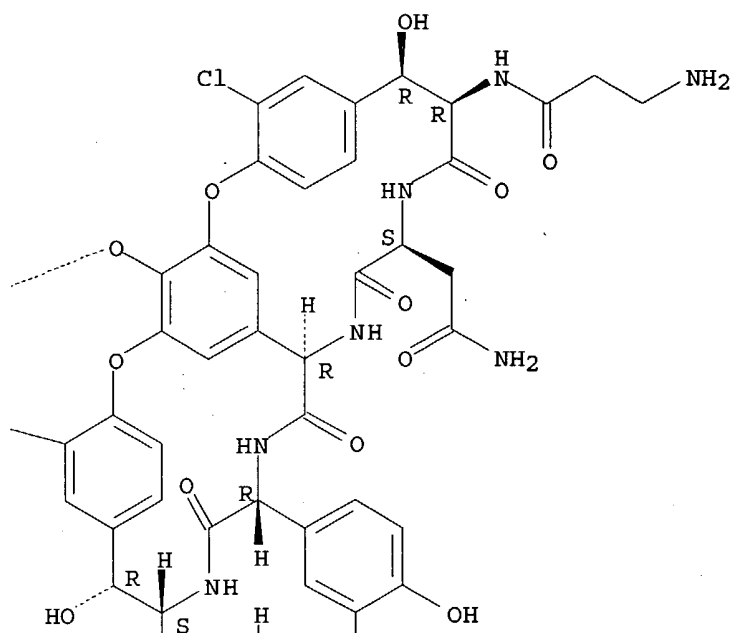
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-(3-amino-1-oxopropyl)-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

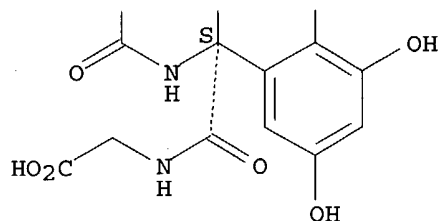
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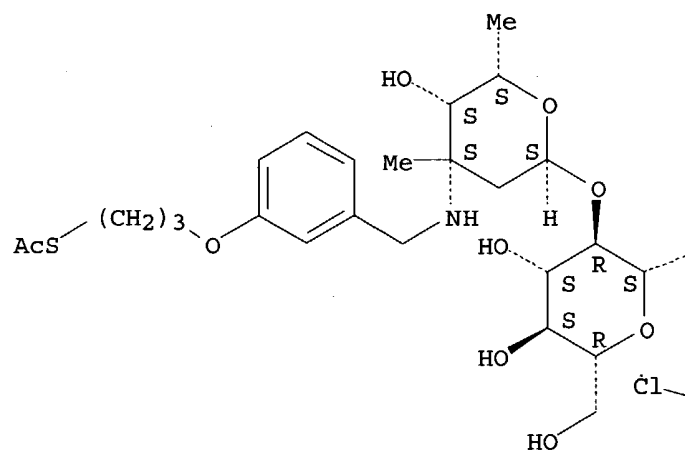


RN 383183-75-3 HCAPLUS

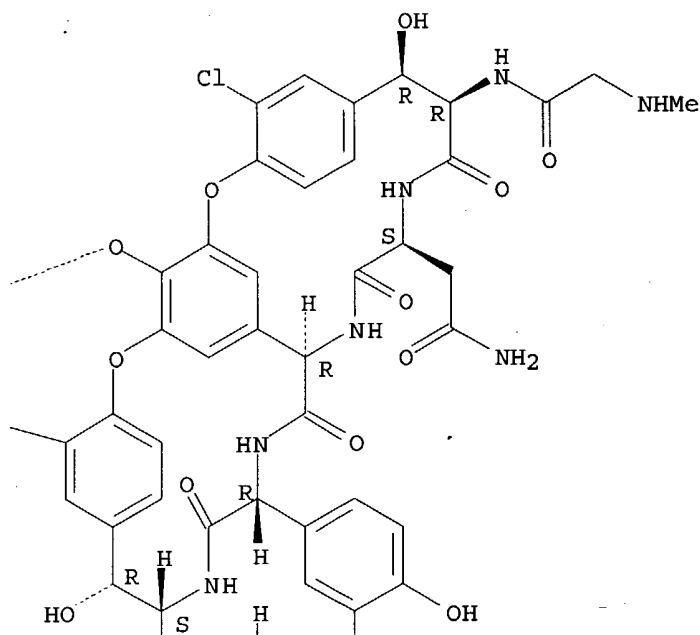
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-28-
 [[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-
 (methylamino)-1-oxopentyl]-49-[(methylamino)acetyl]-(9CI) (CA INDEX
 NAME)

Absolute stereochemistry.

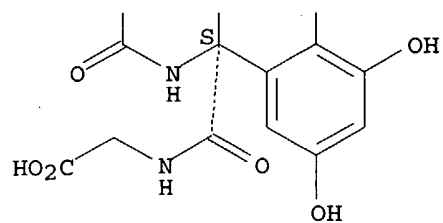
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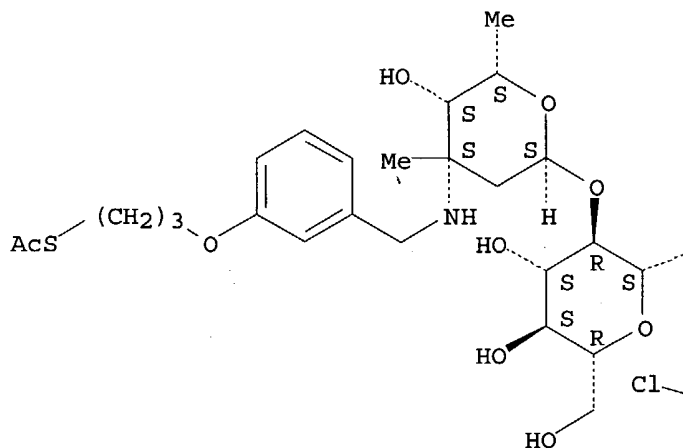


RN 383183-76-4 HCAPLUS

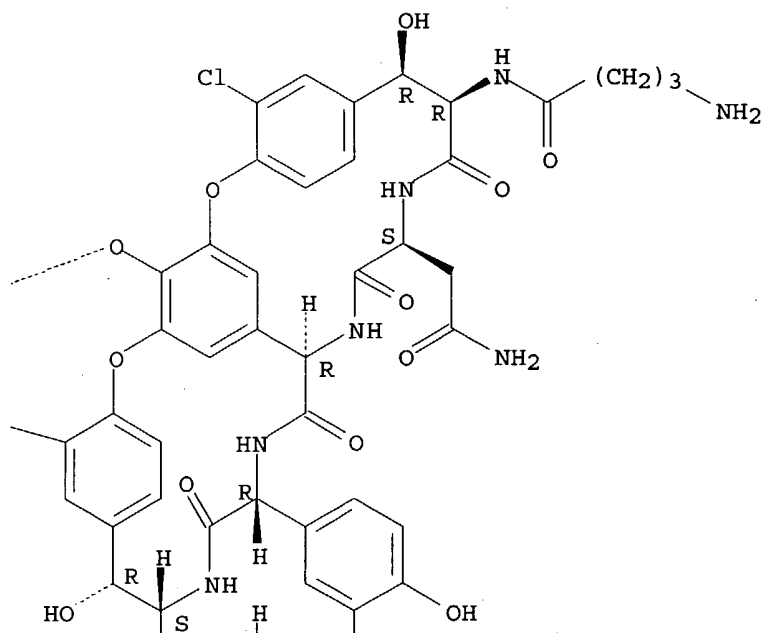
CN Vancomycin, N3''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-(4-amino-1-oxobutyl)-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

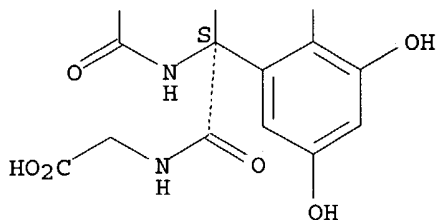
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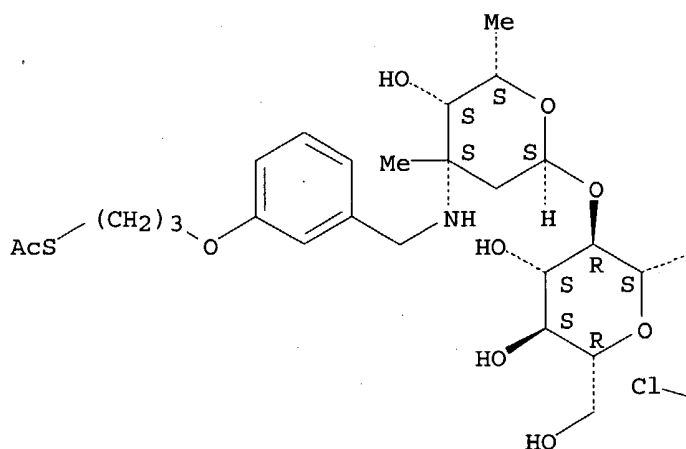


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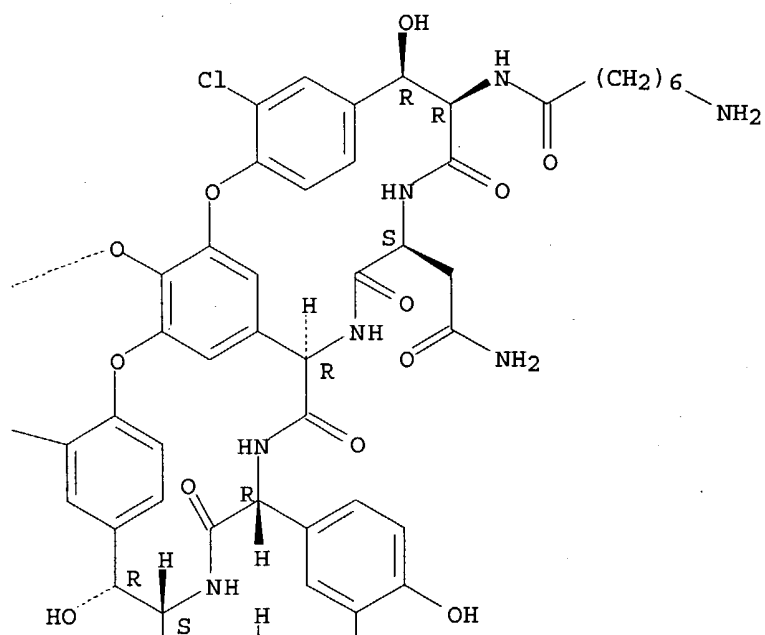
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-(7-amino-1-oxoheptyl)-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

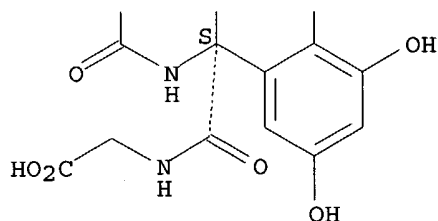
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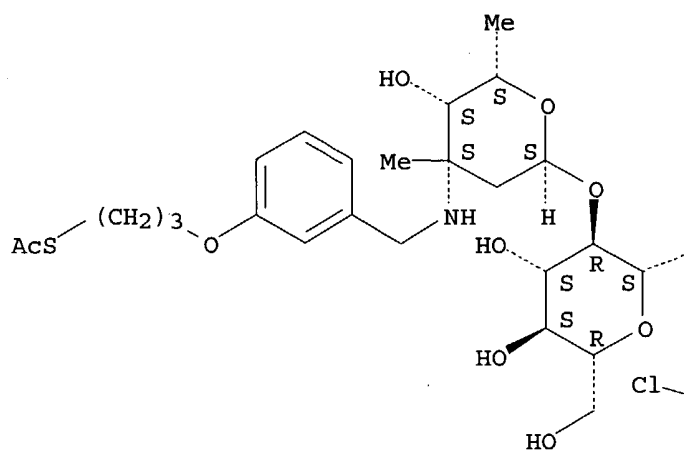


RN 383183-78-6 HCAPLUS

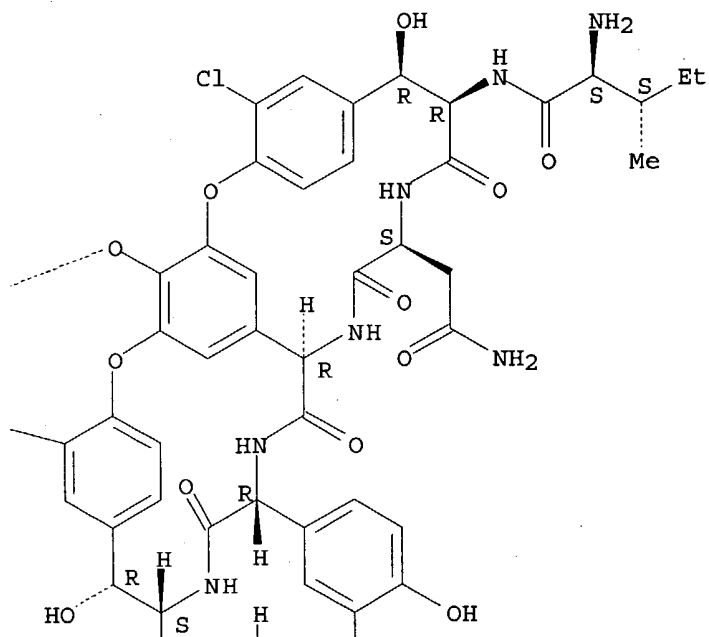
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S,3S)-2-amino-3-methyl-1-oxopentyl]-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

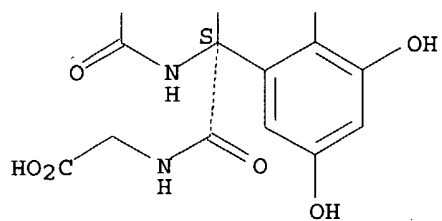
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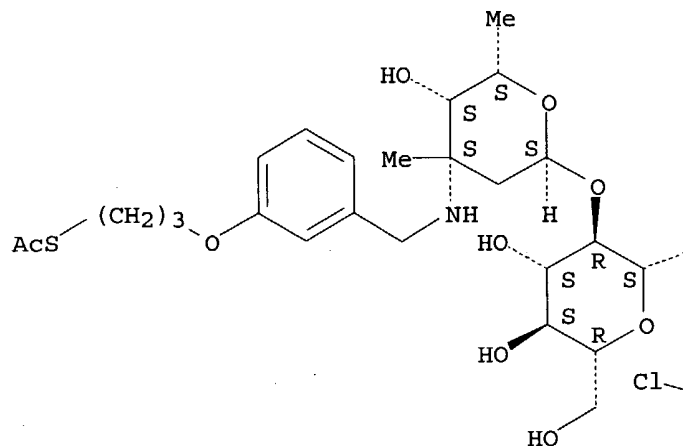


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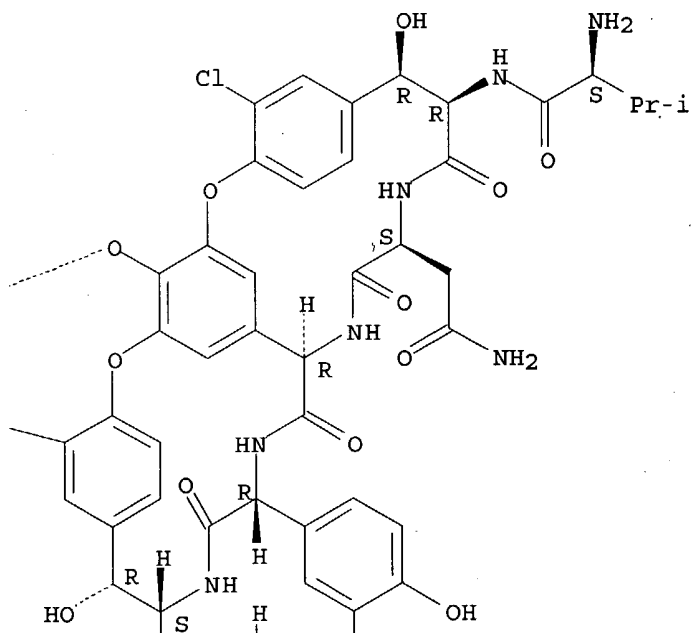
CN Vancomycin, N3'' - [[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-3-methyl-1-oxobutyl]-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

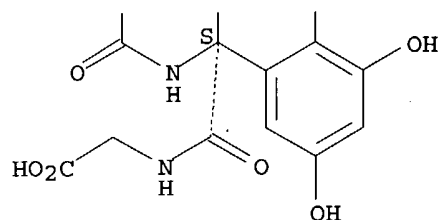
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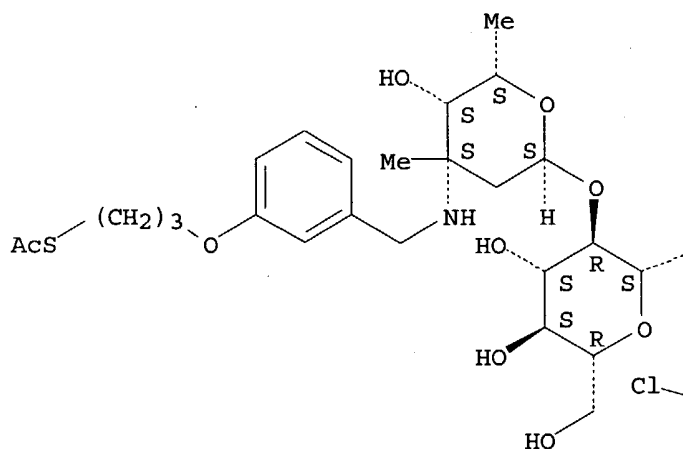


RN 383183-80-0 HCAPLUS

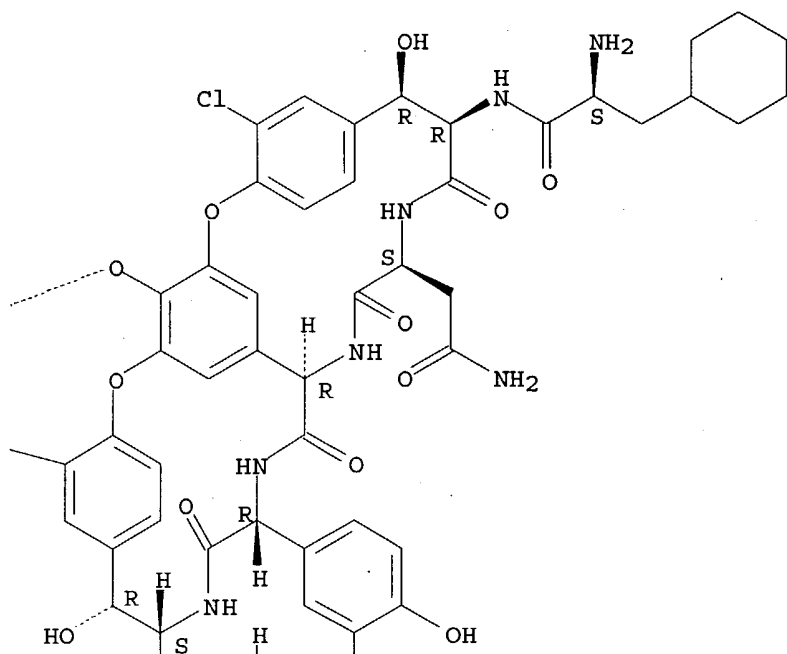
Vancomycin, N3''' - [[3- [3- (acetylthio)propoxy]phenyl]methyl] -49- [(2S) -2- amino-3-cyclohexyl-1-oxopropyl] -28- [[(carboxymethyl)amino]carbonyl] -28- decarboxy-49-de[4-methyl-2- (methylamino) -1-oxopentyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

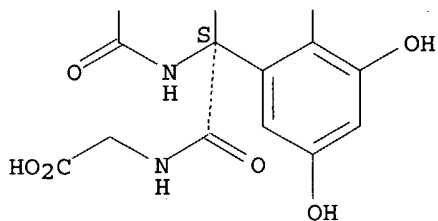
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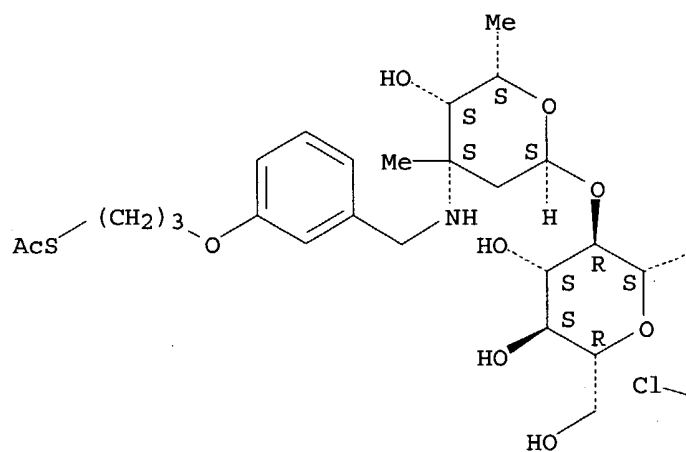


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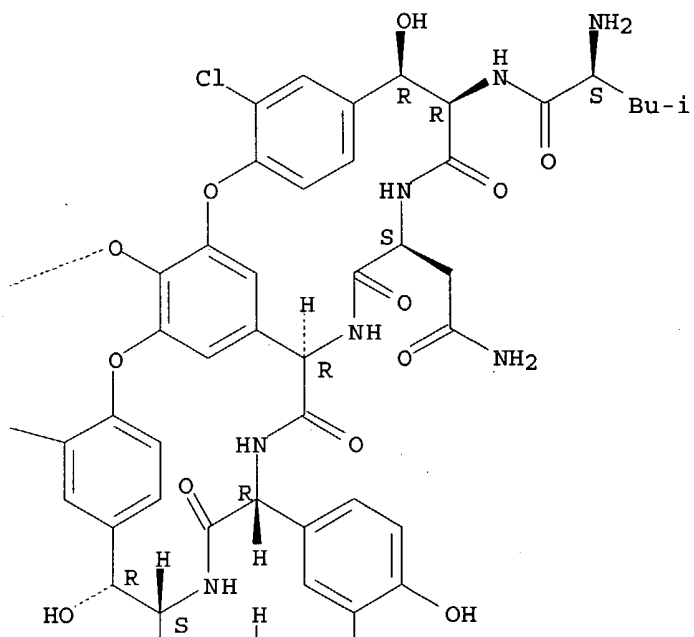
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-28-
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 (CA INDEX NAME)

Absolute stereochemistry.

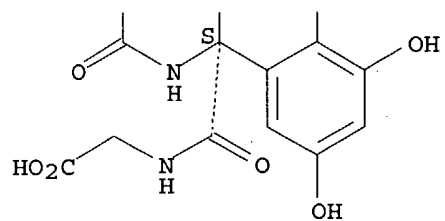
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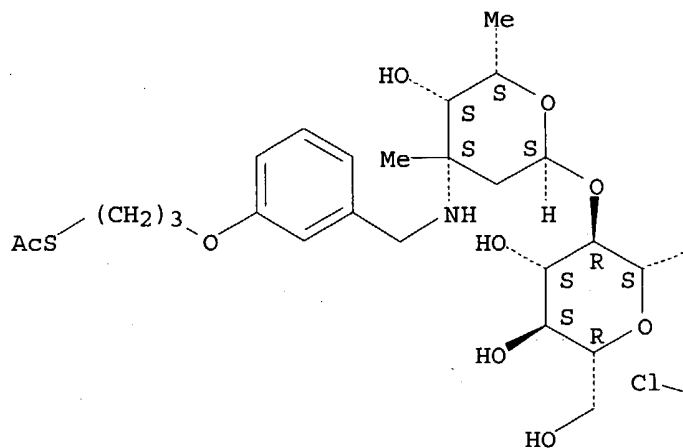


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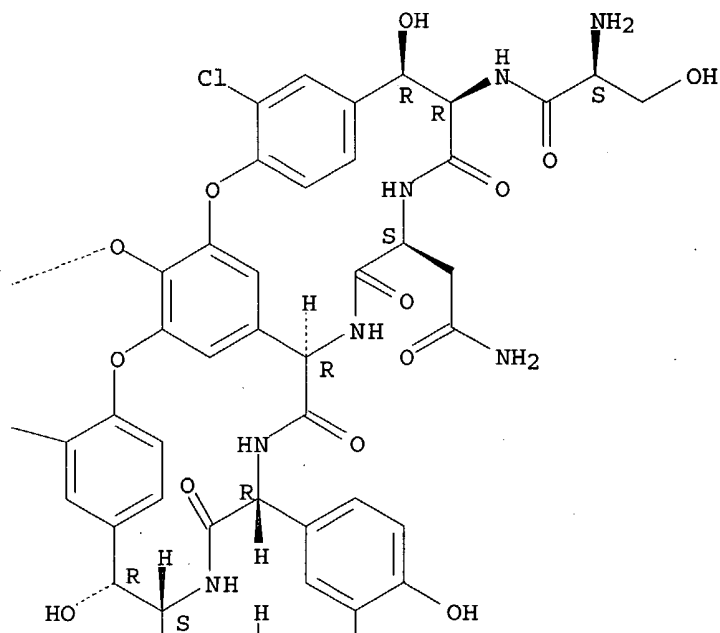
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-3-hydroxy-1-oxopropyl]-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

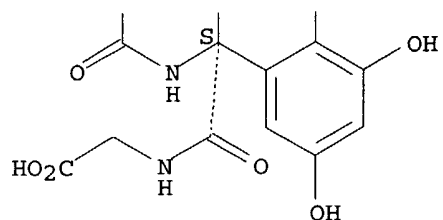
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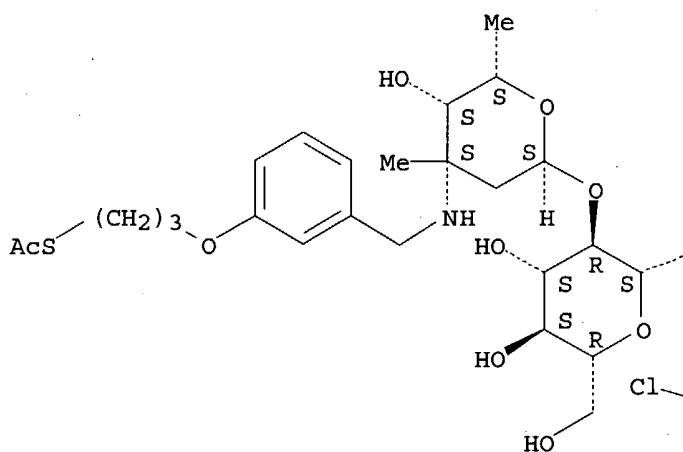


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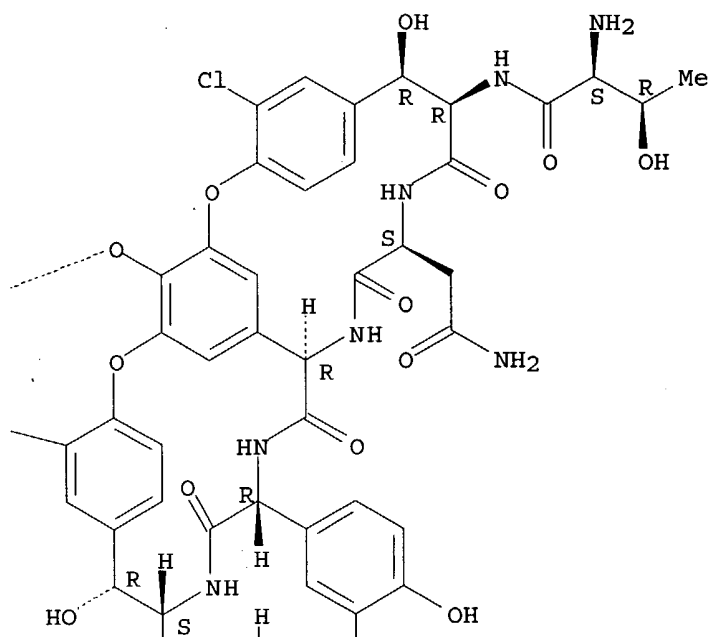
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S,3R)-2-amino-3-hydroxy-1-oxobutyl]-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

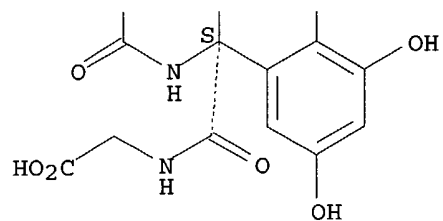
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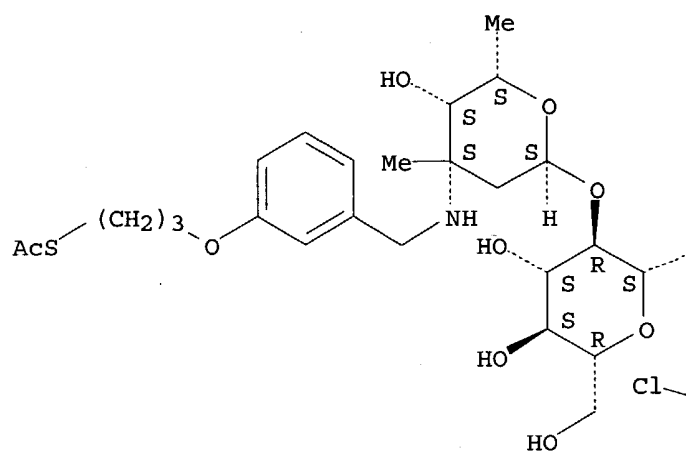


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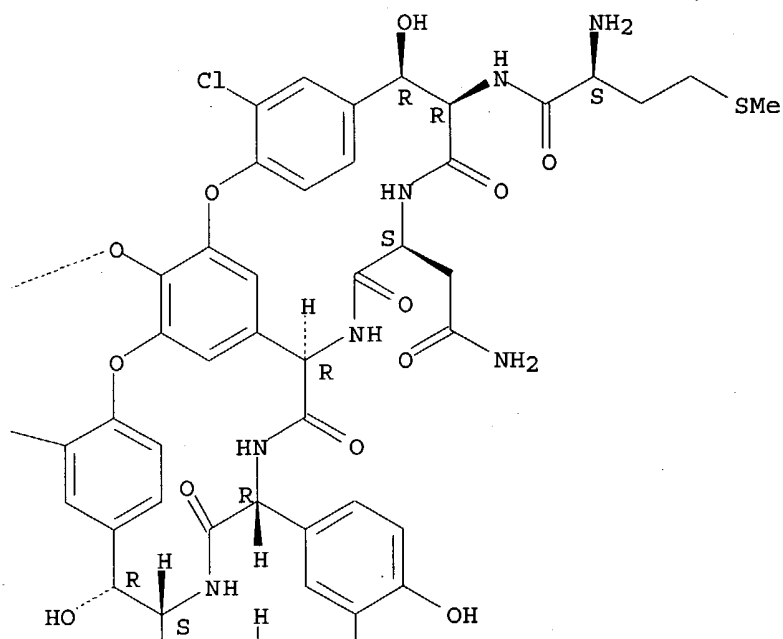
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-4-(methylthio)-1-oxobutyl]-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

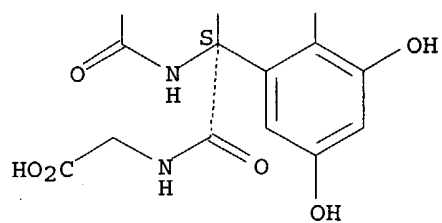
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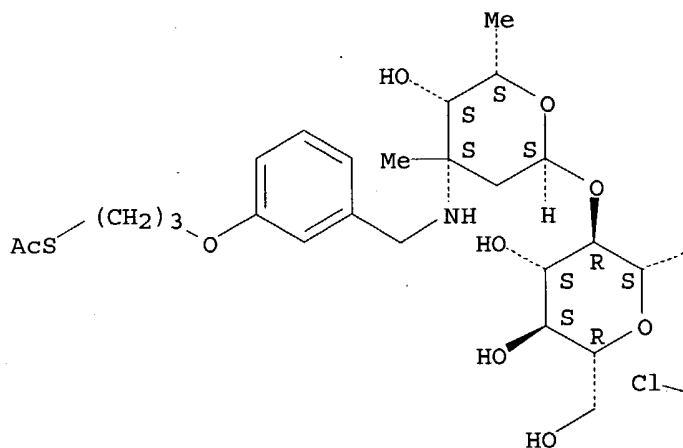
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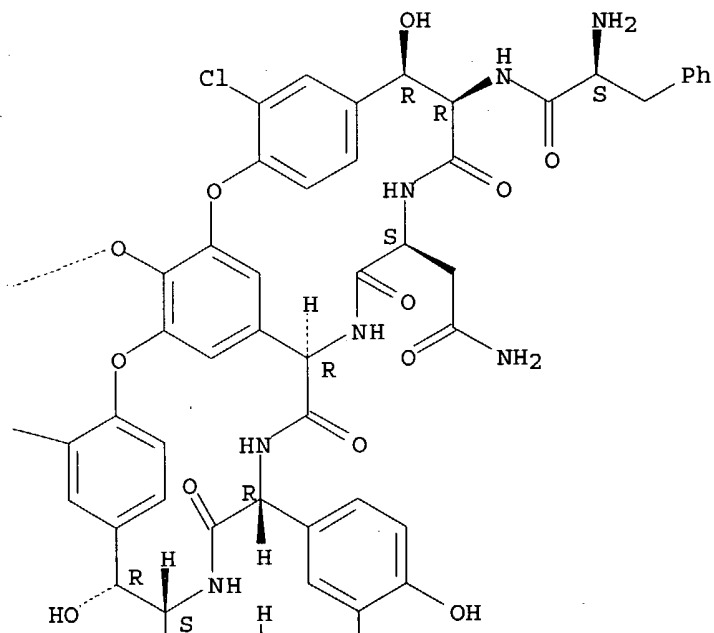
RN 383184-99-4 HCAPLUS
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Absolute stereochemistry.

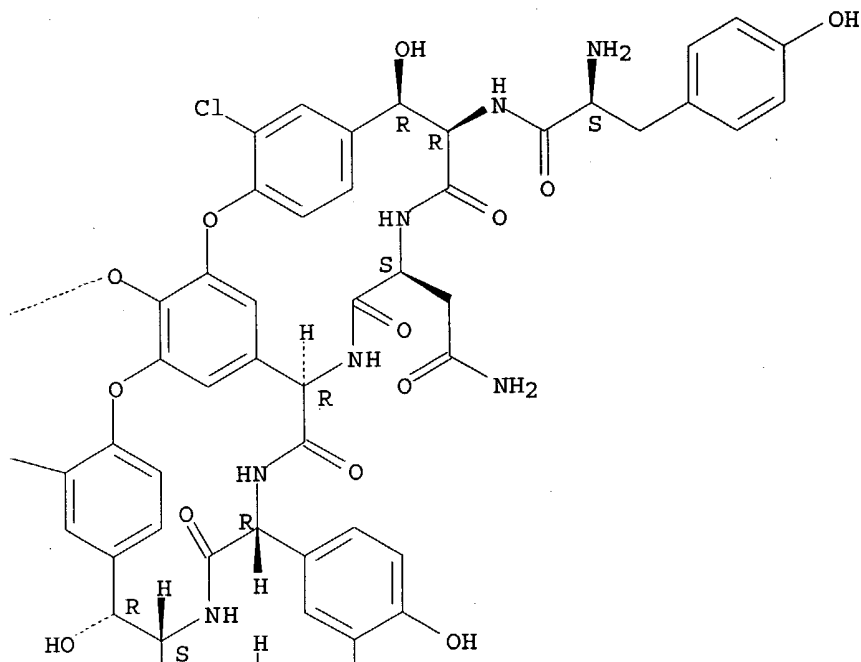
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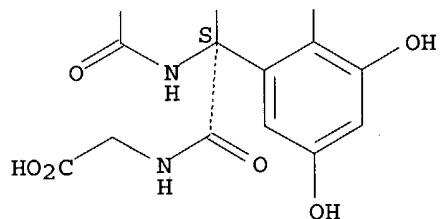
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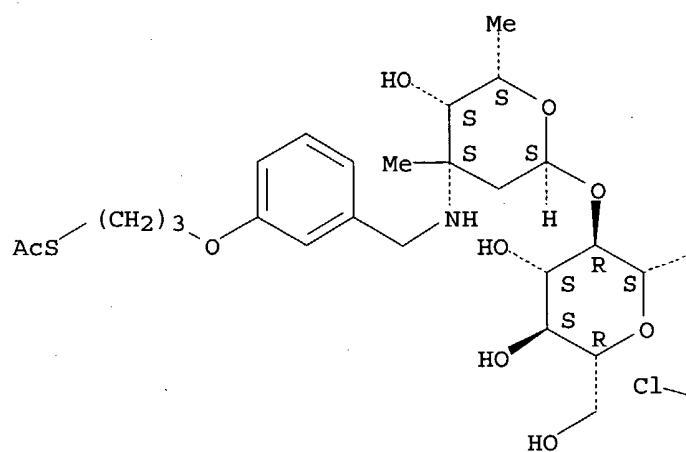
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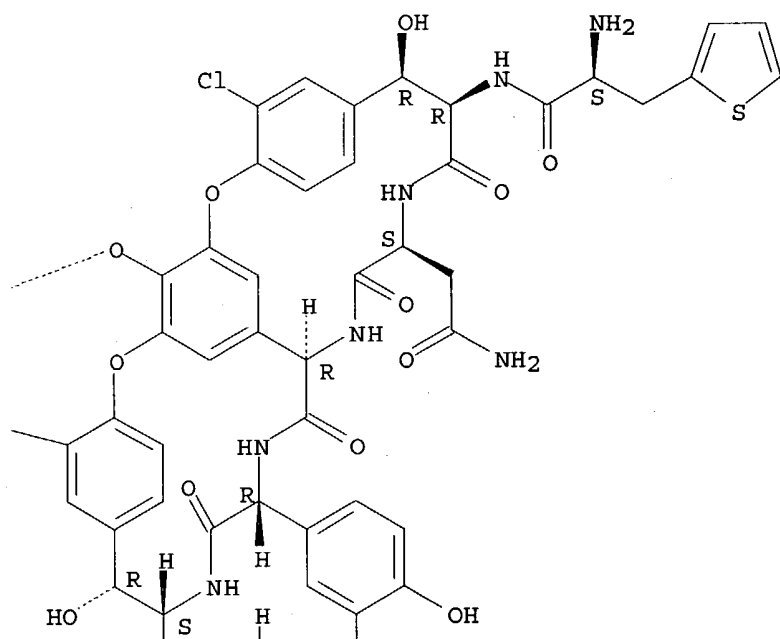
RN 383185-06-6 HCAPLUS
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Absolute stereochemistry.

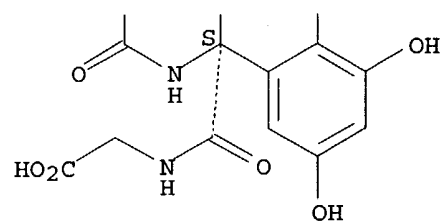
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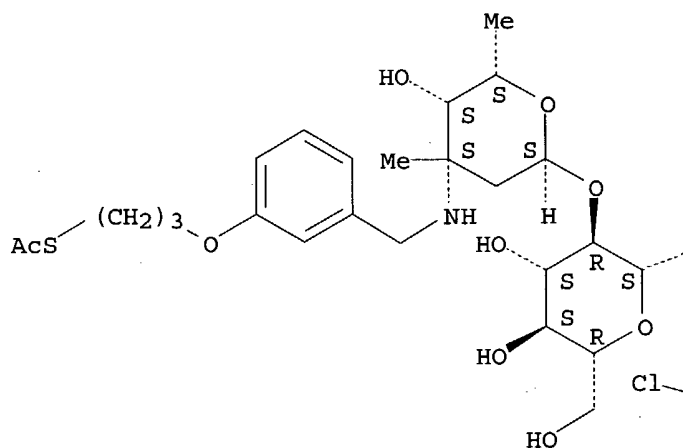


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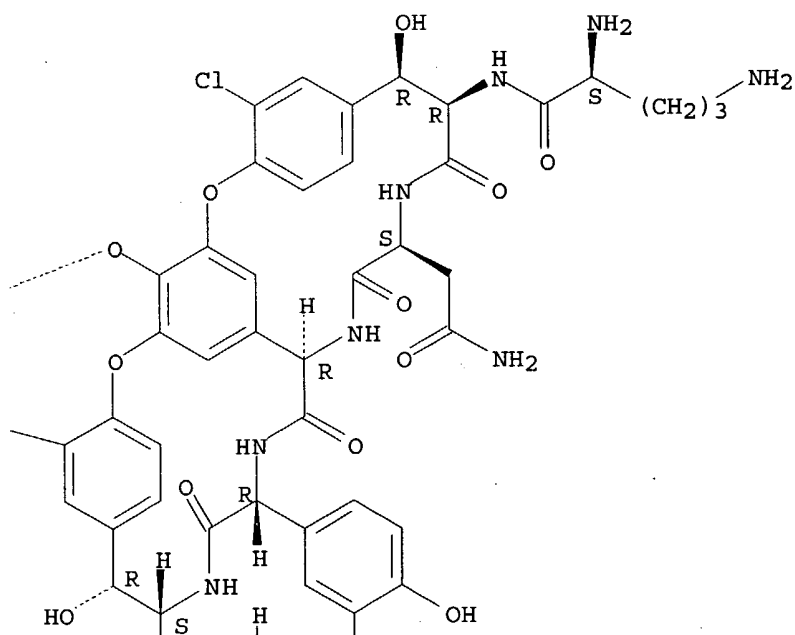
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-54-amino-26-
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INDEX NAME)

Absolute stereochemistry.

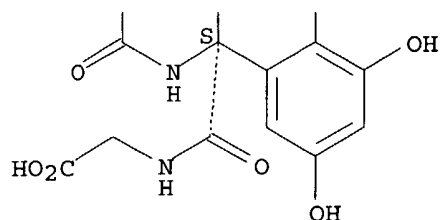
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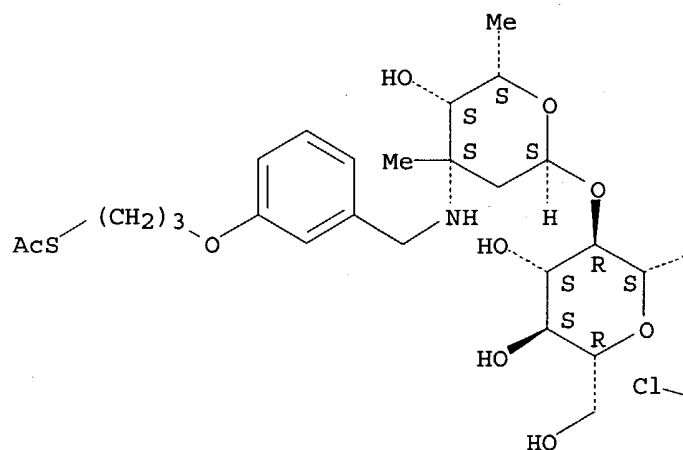


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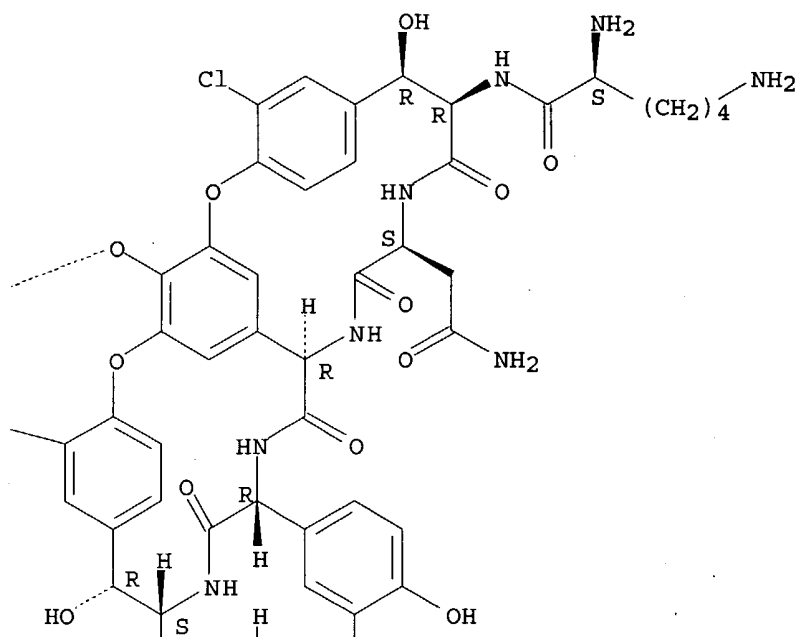
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-26-
 [[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-
 (methylamino)-1-oxopentyl]-49-[(2S)-2,6-diamino-1-oxohexyl]- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.

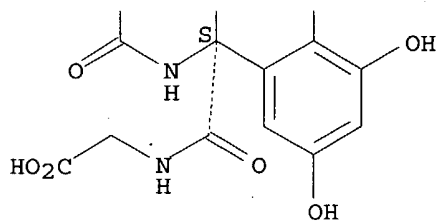
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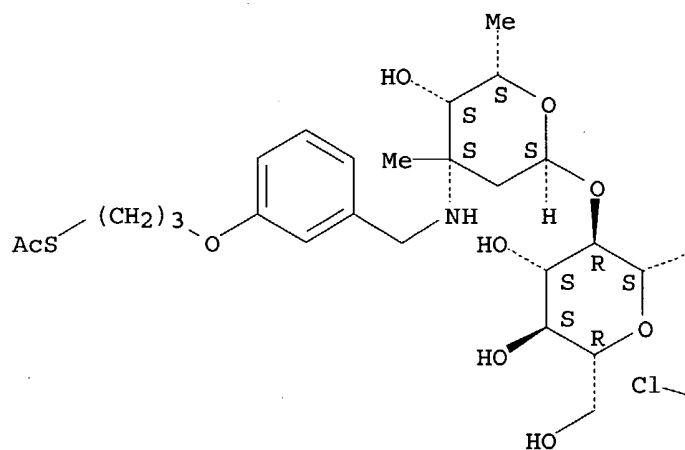


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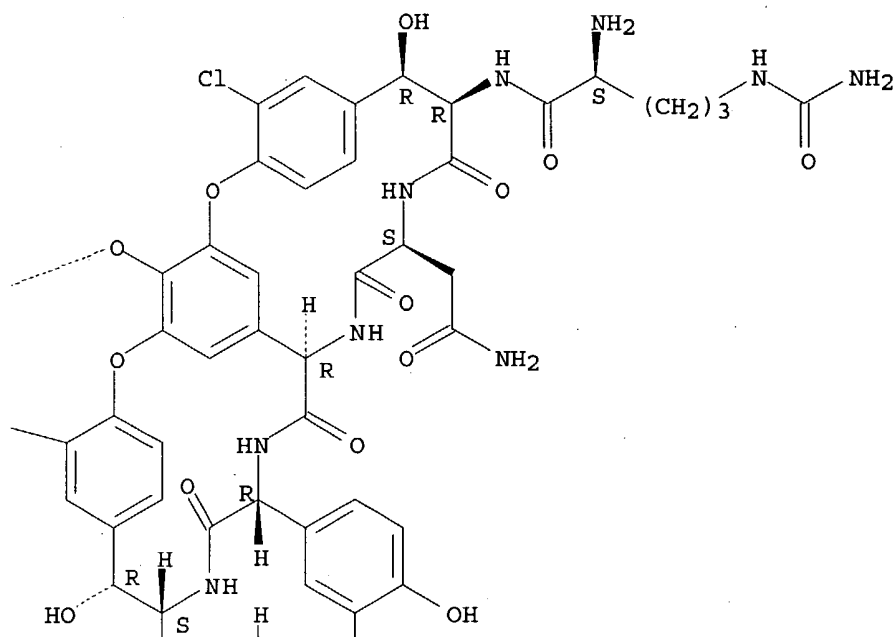
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-54-
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Absolute stereochemistry.

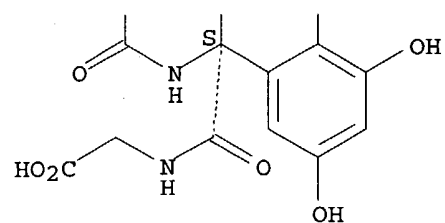
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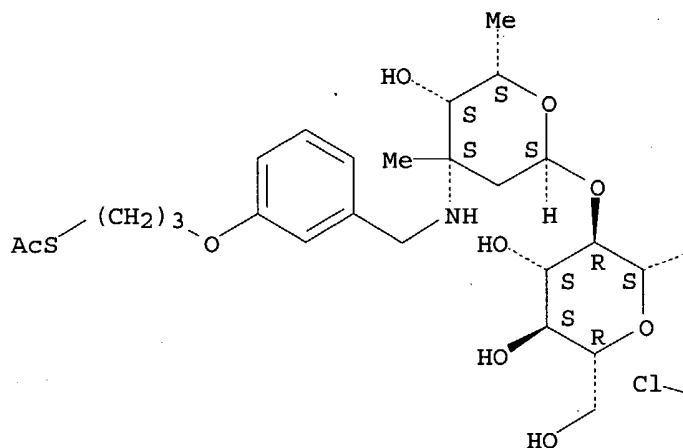
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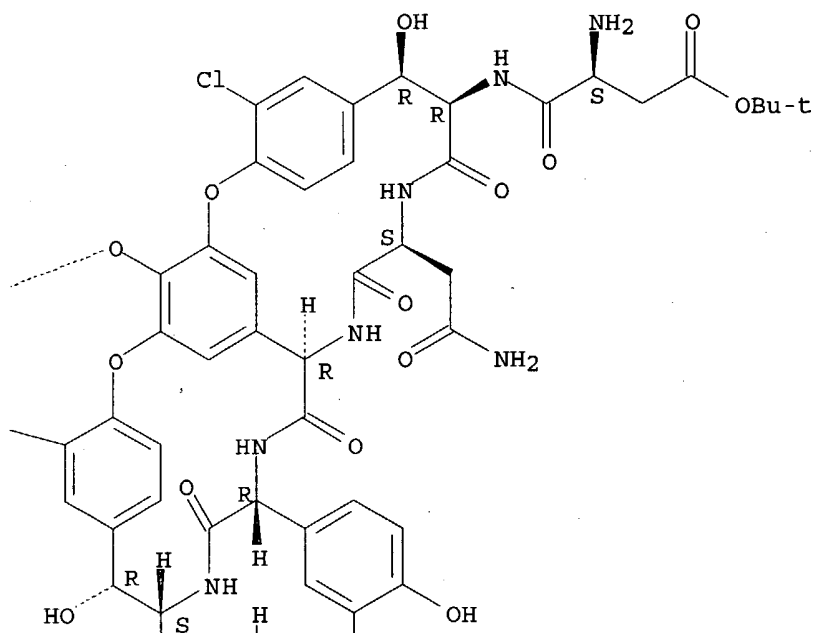
RN 383185-12-4 HCAPLUS
CN Vancomycin, N3''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-4-(1,1-dimethylethoxy)-1,4-dioxobutyl]-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

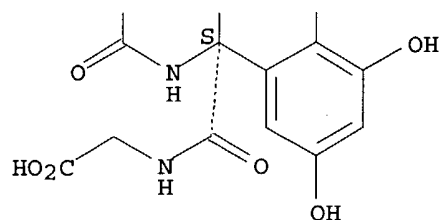
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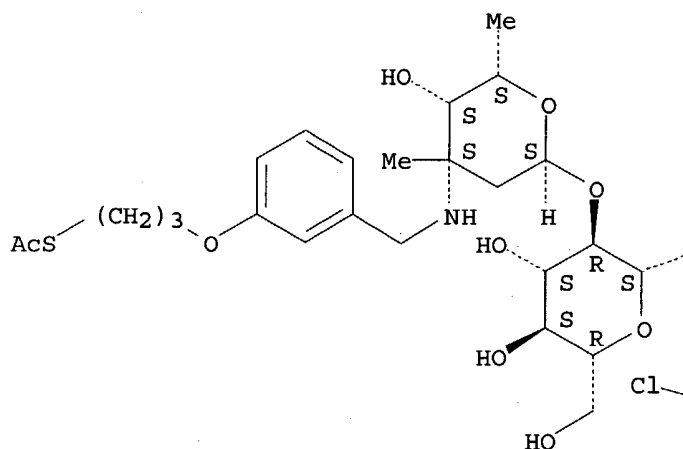


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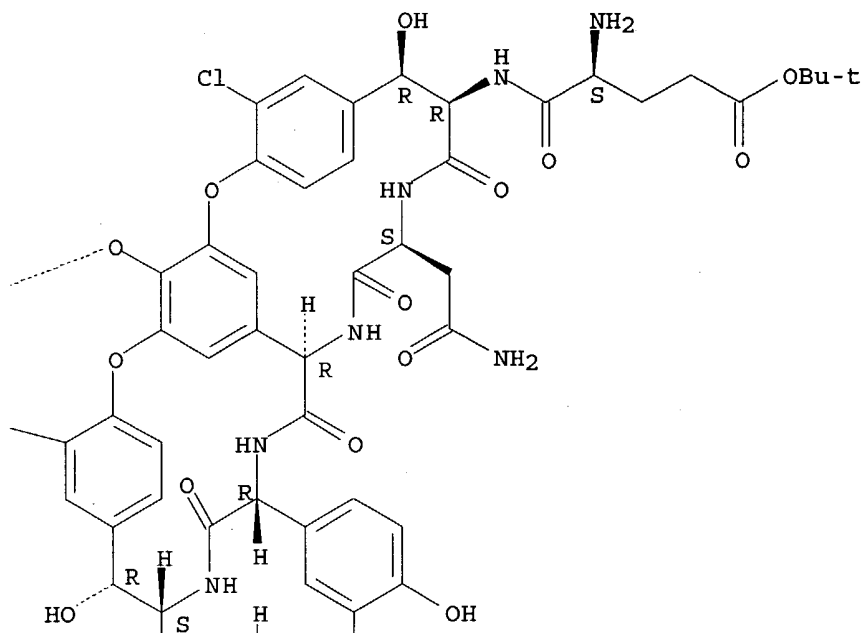
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-54-(1,1-dimethylethoxy)-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-53,56-didemethyl-54-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

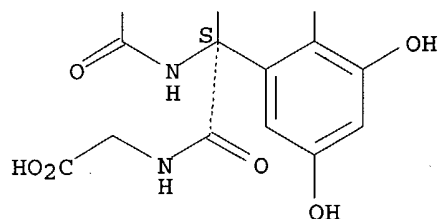
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L65 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 2001:689110 HCAPLUS
 DN 136:70059
 ED Entered STN: 20 Sep 2001
 TI Solid- and solution-phase synthesis of vancomycin and vancomycin analogues with activity against vancomycin-resistant bacteria
 AU Nicolaou, K. C.; Cho, Suk Young; Hughes, Robert; Winssinger, Nicolas; Smethurst, Christian; Labischinski, Harald; Endermann, Rainer
 CS Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
 SO Chemistry--A European Journal (2001), 7(17), 3798-3823
 CODEN: CEUJED; ISSN: 0947-6539
 PB Wiley-VCH Verlag GmbH
 DT Journal
 LA English
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 1, 33
 AB Vancomycin, the prototypical member of the glycopeptide family of antibiotics, is a clin. used antibiotic employed against a variety of drug-resistant bacterial strains including methicillin-resistant *Staphylococcus aureus* (MRSA). The recent emergence of vancomycin

resistance, viewed as a growing threat to public health, prompted us to initiate a program aimed at restoring the potency of this important antibiotic through chemical manipulation of the vancomycin structure. We describe the development of synthetic technol. based on the design of a novel selenium safety catch linker, application of this technol. to a solid-phase semisynthesis of vancomycin, and the solid- and solution-phase synthesis of vancomycin libraries. Biol. evaluation of these compound libraries led to the identification of a number of in vitro highly potent antibacterial agents effective against vancomycin-resistant bacteria. In addition to aiding these investigations, the solid-phase chemical described herein is expected to enhance the power of combinatorial chemical and facilitate chemical biol. and medicinal chemical studies.

- ST vancomycin analog synthesis antibacterial; selenium safety catch linker
solid phase synthesis vancomycin analog
- IT Solid phase synthesis
(peptide; selenium safety catch linker in synthesis of vancomycin and vancomycin analogs with activity against vancomycin-resistant bacteria)
- IT Antibacterial agents
Antibiotics
Peptide library
(synthesis of vancomycin and vancomycin analogs with activity against vancomycin-resistant bacteria)
- IT Glycopeptides
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of vancomycin and vancomycin analogs with activity against vancomycin-resistant bacteria)
- IT 383183-30-0 383183-31-1 383183-32-2
383183-33-3 383183-34-4 383183-35-5
383183-36-6 383183-37-7 383183-38-8
383183-39-9 383183-40-2 383183-41-3
383183-45-7 383183-46-8 383183-76-4
383424-20-2 383424-21-3 383424-22-4 383424-23-5 383424-24-6
383424-25-7 383424-26-8 383424-27-9
RL: PAC (Pharmacological activity); BIOL (Biological study)
(synthesis of vancomycin and vancomycin analogs with activity against vancomycin-resistant bacteria)
- IT 321361-97-1P 321362-17-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of vancomycin and vancomycin analogs with activity against vancomycin-resistant bacteria)
- IT 1404-90-6DP, Vancomycin, analogs 119728-56-2P 321361-99-3P
321362-01-0P 321362-05-4P 321362-07-6P 321362-09-8P 321362-11-2P
321362-13-4P 383183-42-4P 383183-43-5P
383183-44-6P 383183-71-9P 383183-72-0P
383183-74-2P 383183-75-3P 383183-78-6P
383183-79-7P 383183-80-0P 383183-81-1P
383183-82-2P 383184-29-0P 383184-31-4P 383184-33-6P
383184-34-7P 383184-36-9P 383184-39-2P 383184-41-6P 383184-43-8P
383184-45-0P 383184-47-2P 383184-53-0P 383184-56-3P 383184-58-5P
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383424-65-5P 383424-66-6P 383424-67-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
(Biological study); PREP (Preparation)

(synthesis of vancomycin and vancomycin analogs with activity against
vancomycin-resistant bacteria)

IT 100-51-6, Benzenemethanol, reactions 100-83-4 103-72-0,
Phenylthioisocyanate 107-18-6, 2-Propen-1-ol, reactions 111-87-5,
1-Octanol, reactions 112-30-1, 1-Decanol 123-08-0,
4-Hydroxybenzaldehyde 139-85-5, 3,4-Dihydroxybenzaldehyde 507-09-5,
Thiolacetic acid, reactions 627-27-0, 3-Buten-1-ol 627-31-6,
1,3-Diiodopropane 821-09-0, 4-Penten-1-ol 821-41-0, 5-Hexen-1-ol
873-76-7 1404-93-9, Vancomycin hydrochloride 13019-22-2, 9-Decen-1-ol
14002-51-8, [1,1'-Biphenyl]-4-carbonyl chloride 17746-05-3, Undecanoyl
chloride 133754-40-2D, Selenohypobromous acid, resin-bound 221182-36-1
273736-70-2 383423-48-1 383423-49-2 383423-50-5 383423-51-6
383423-52-7 383423-53-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis of vancomycin and vancomycin analogs with activity against
vancomycin-resistant bacteria)

IT 1404-90-6P, Vancomycin 4049-39-2P 40359-32-8P 40663-68-1P
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214847-86-6P 221182-45-2P 250290-69-8P 255047-42-8P 273736-58-6P
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resin-bound 273736-71-3DP, resin-bound 273736-72-4DP, resin-bound
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resin-bound 383423-60-7DP, resin-bound 383423-72-1DP, resin-bound
383423-73-2DP, resin-bound 383423-74-3DP, resin-bound 383423-75-4DP,
resin-bound 383423-76-5DP, resin-bound 383423-77-6DP, resin-bound
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383423-84-5P 383423-85-6P 383423-87-8P 383423-88-9P 383423-90-3P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(synthesis of vancomycin and vancomycin analogs with activity against
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383424-15-5P **383424-30-4P** 383424-68-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of vancomycin and vancomycin analogs with activity against
vancomycin-resistant bacteria)

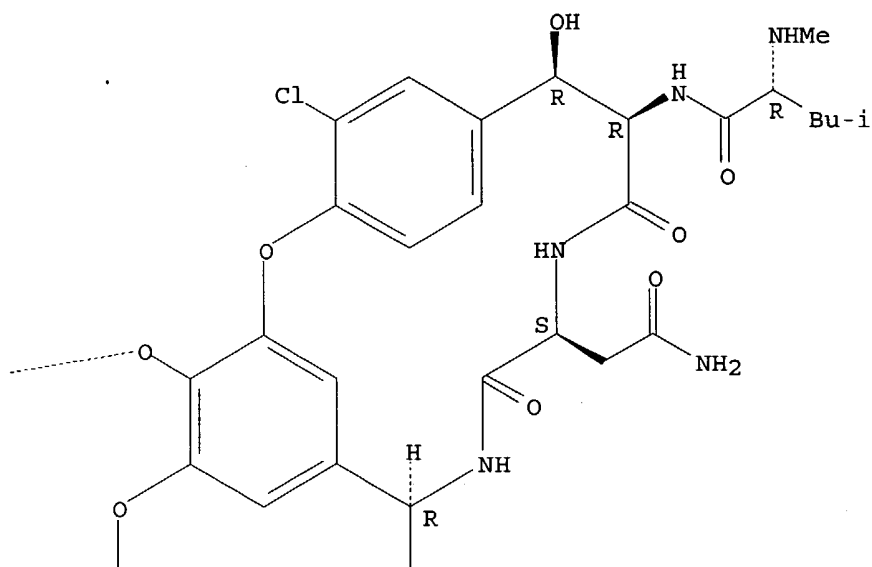
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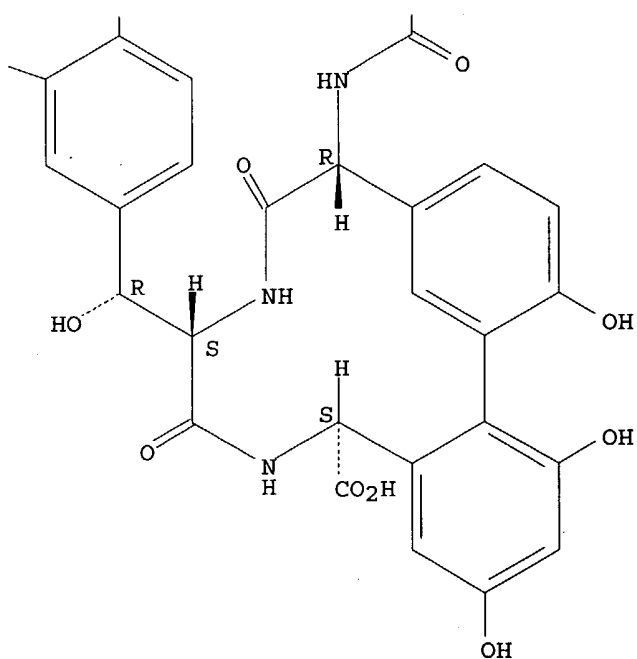
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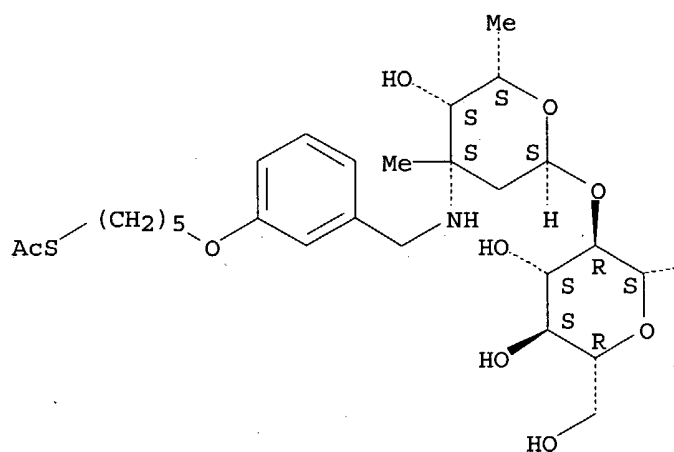


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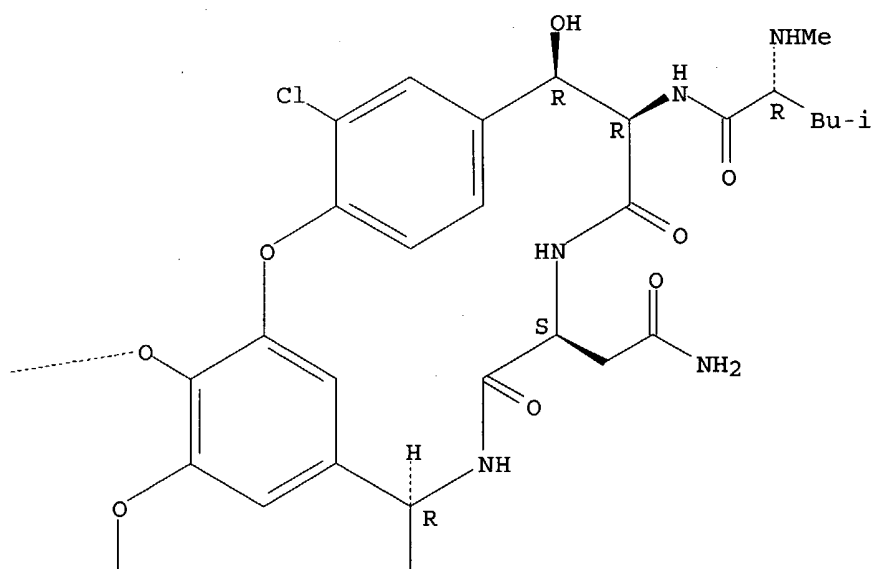
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INDEX NAME)

Absolute stereochemistry.

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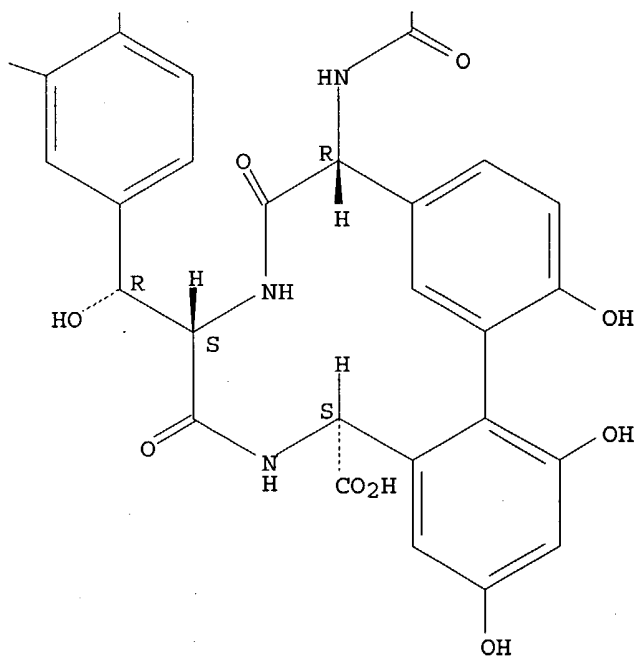
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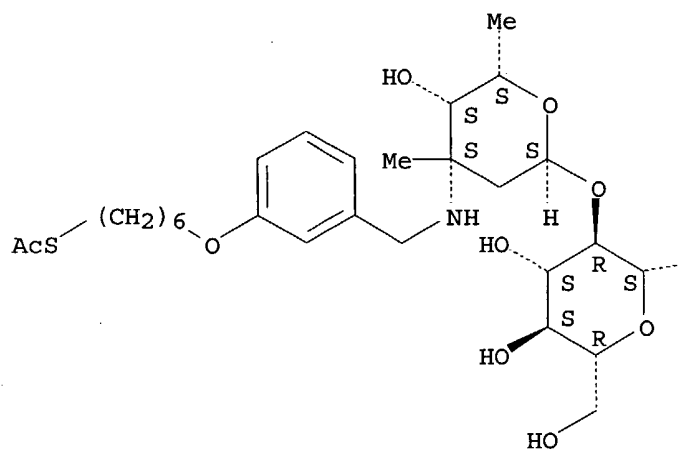


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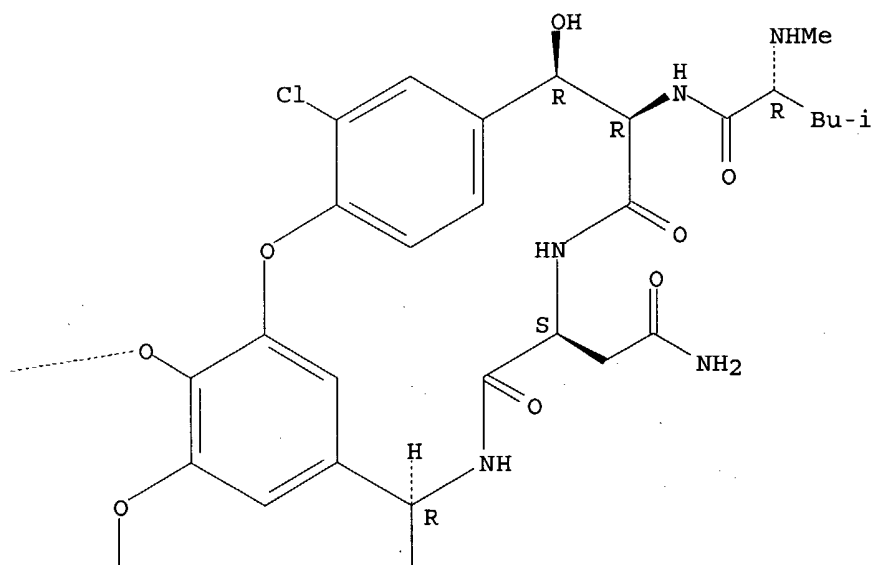
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Absolute stereochemistry.

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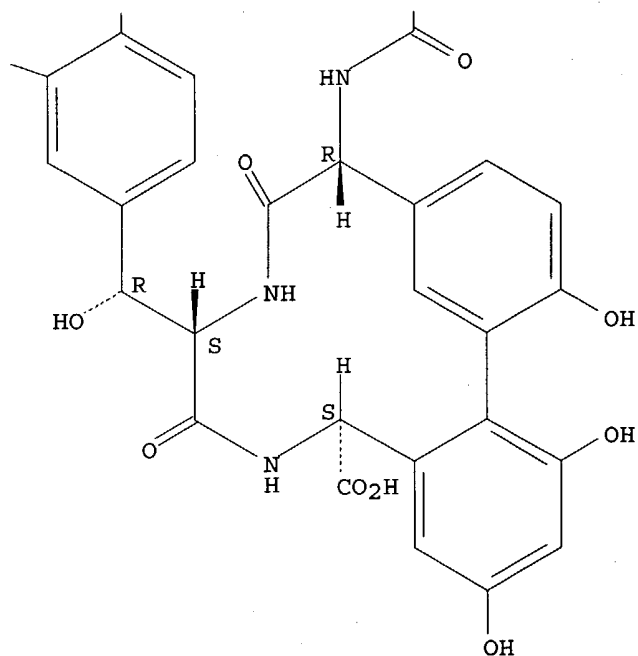
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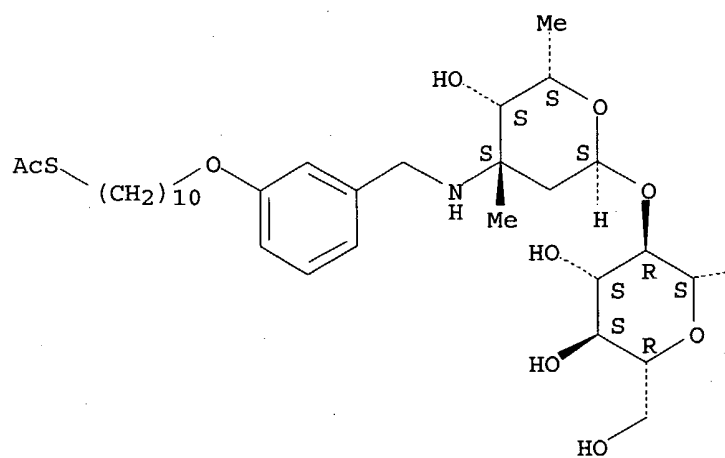


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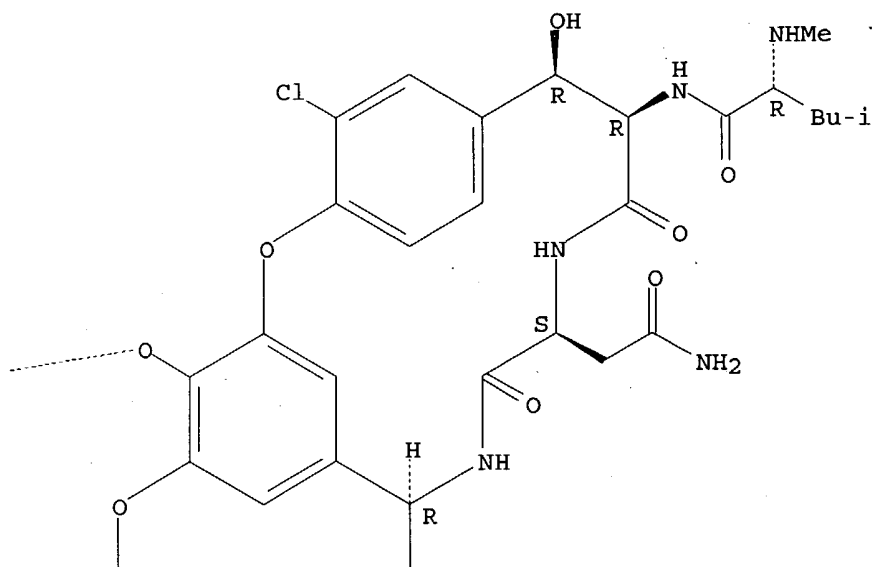
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Absolute stereochemistry.

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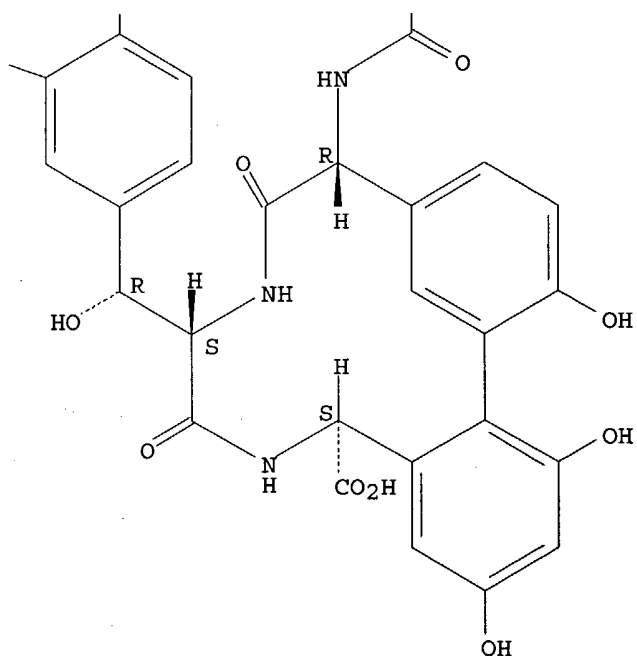
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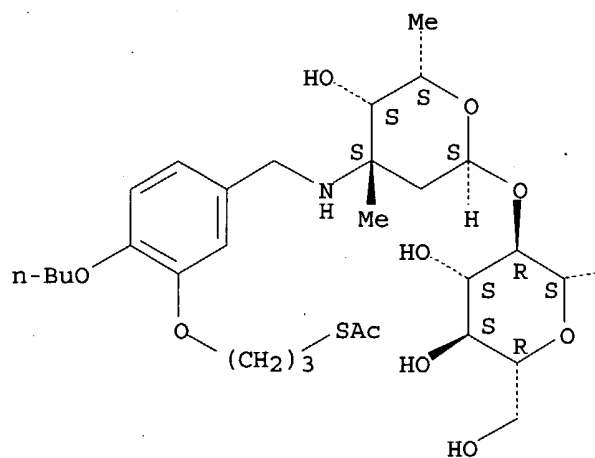


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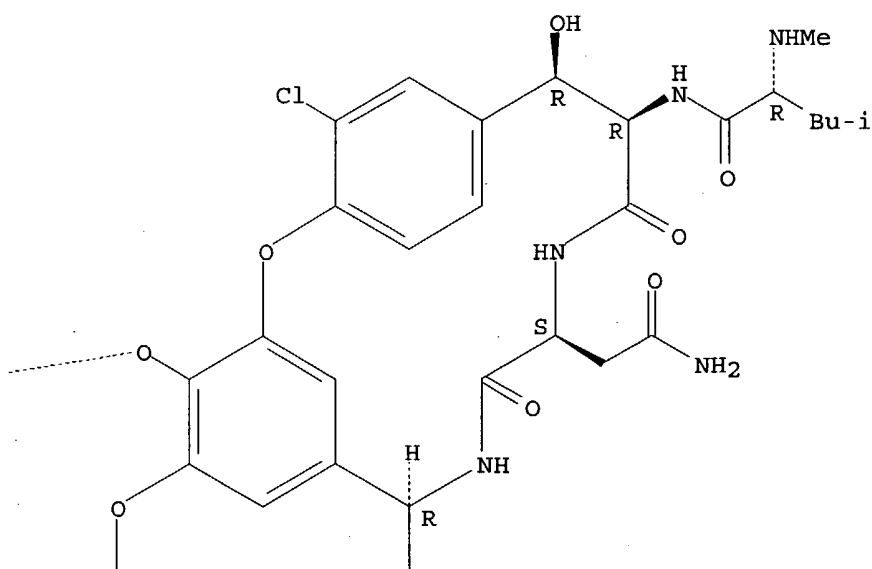
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(CA INDEX NAME)

Absolute stereochemistry.

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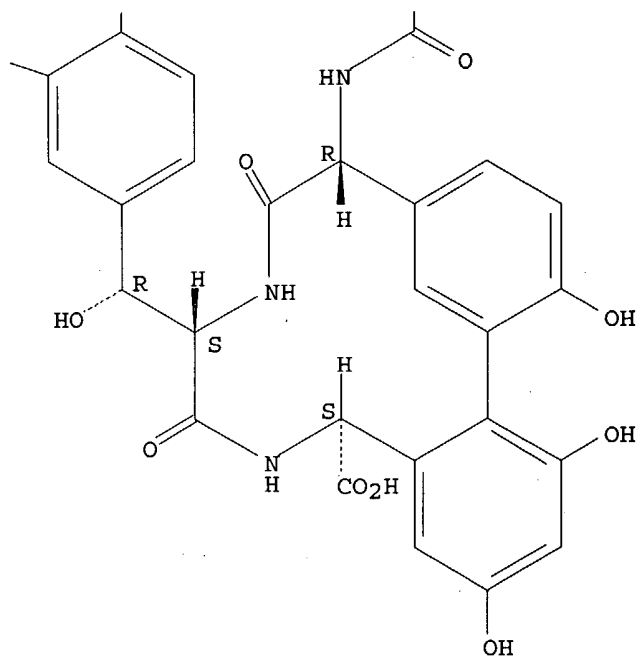
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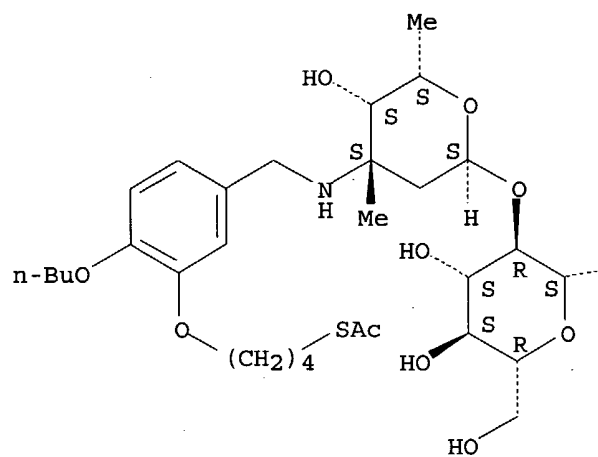


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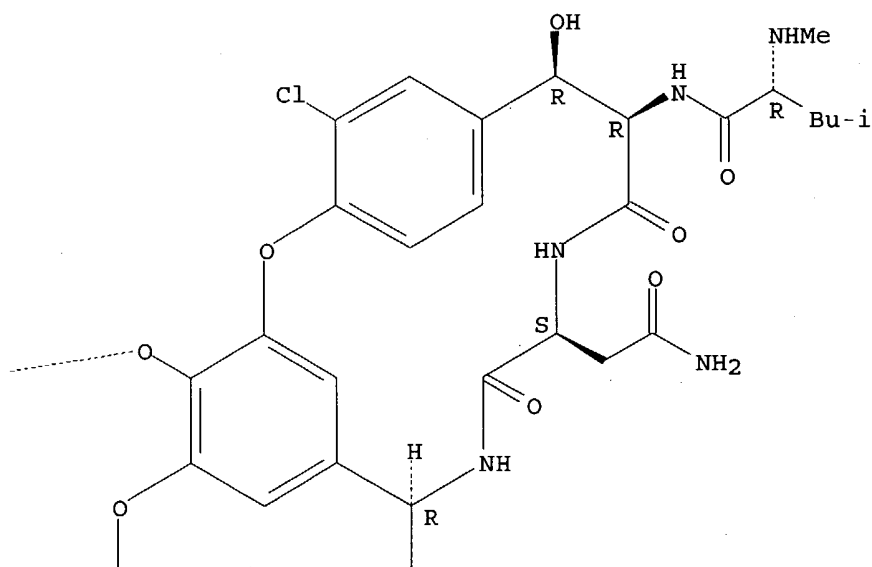
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(CA INDEX NAME)

Absolute stereochemistry.

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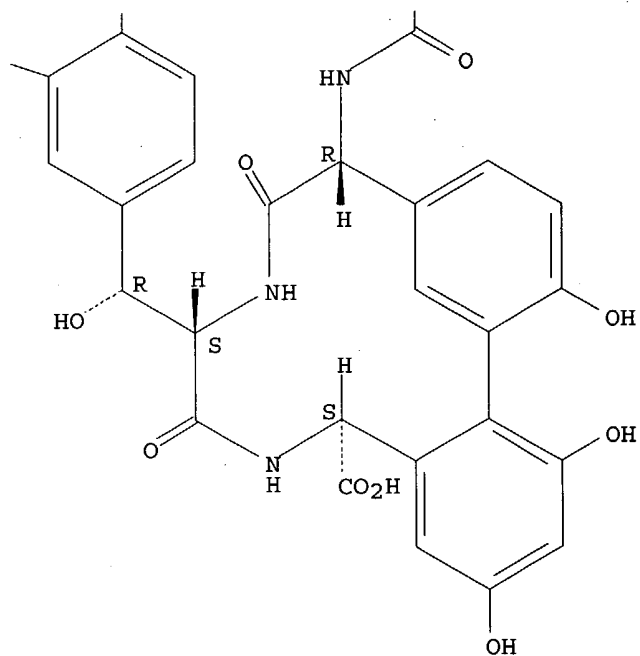
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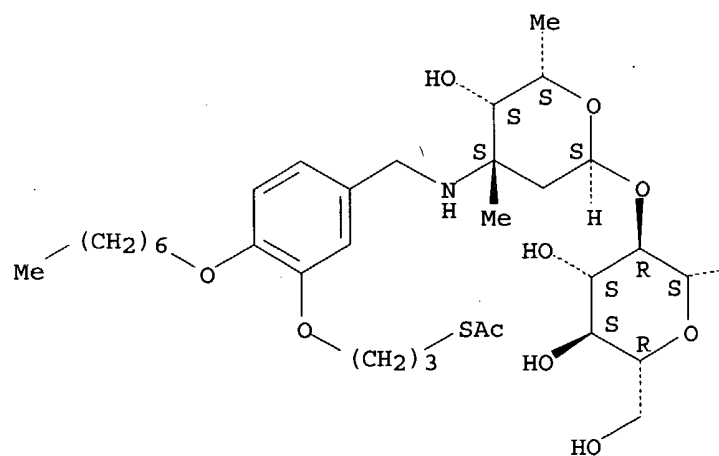


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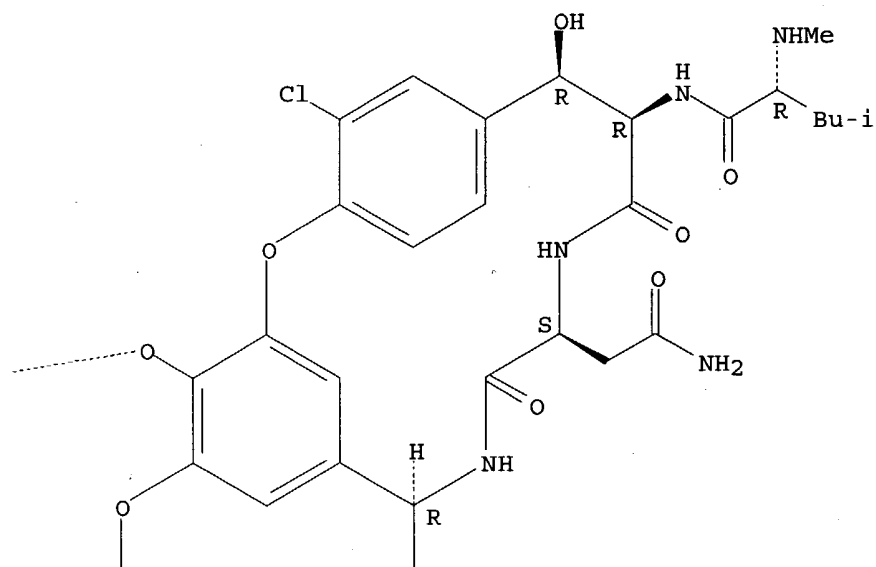
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]-4-(heptyloxy)phenyl]methyl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

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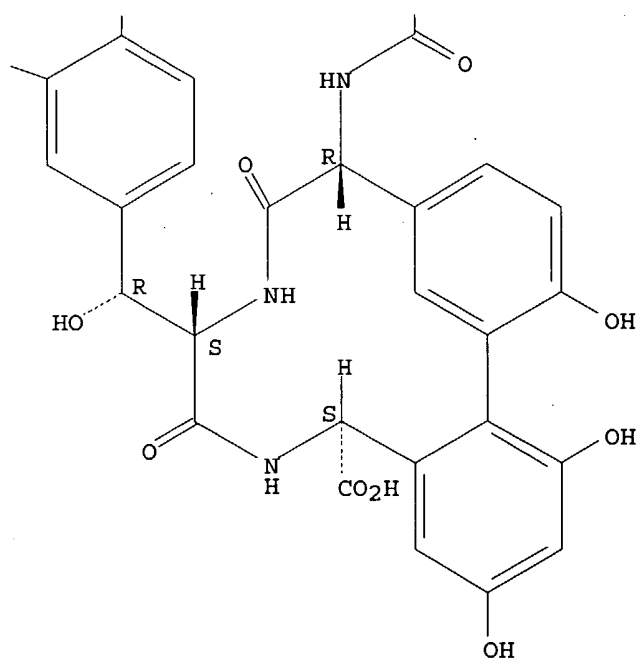
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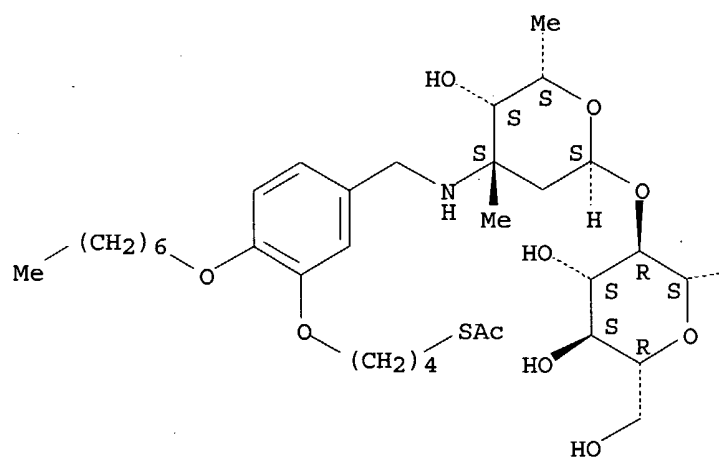


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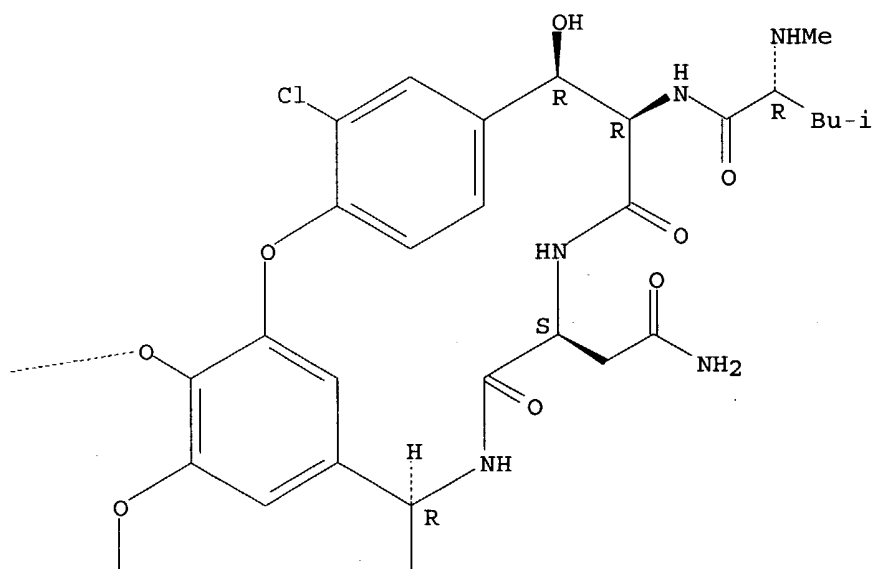
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(9CI) (CA INDEX NAME)

Absolute stereochemistry.

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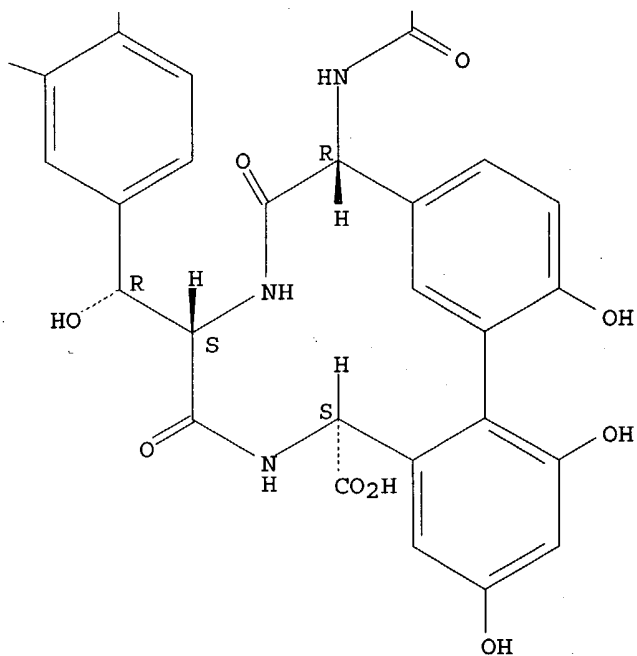
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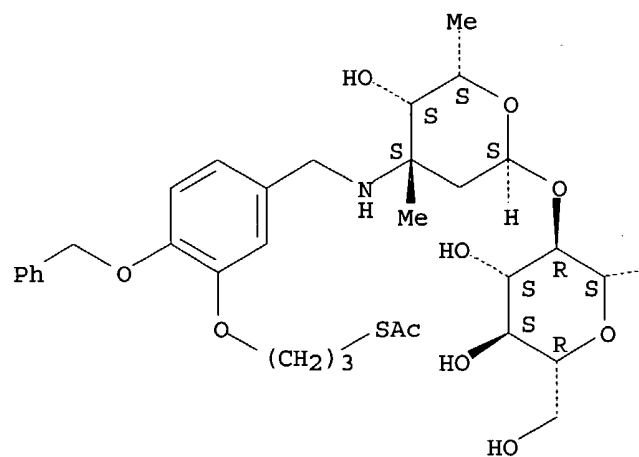


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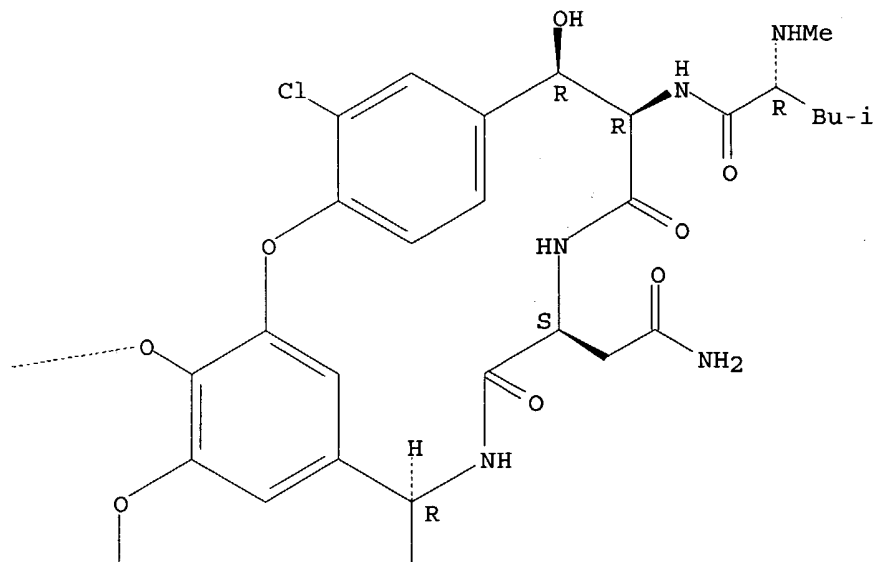
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]-4-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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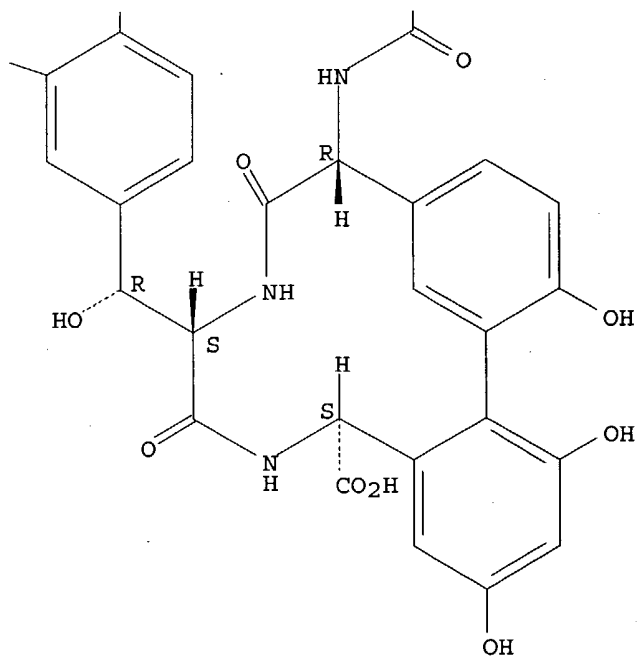
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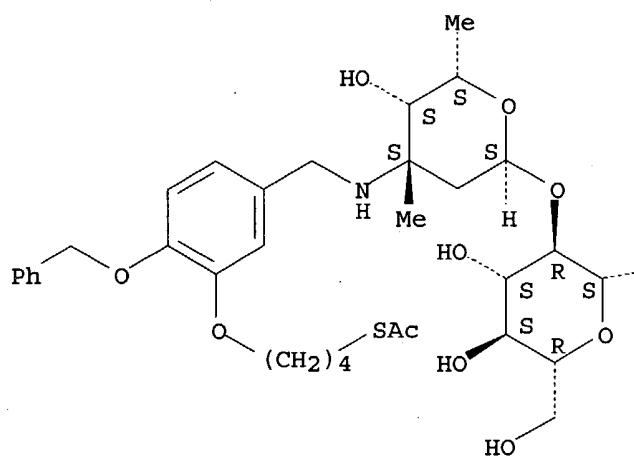


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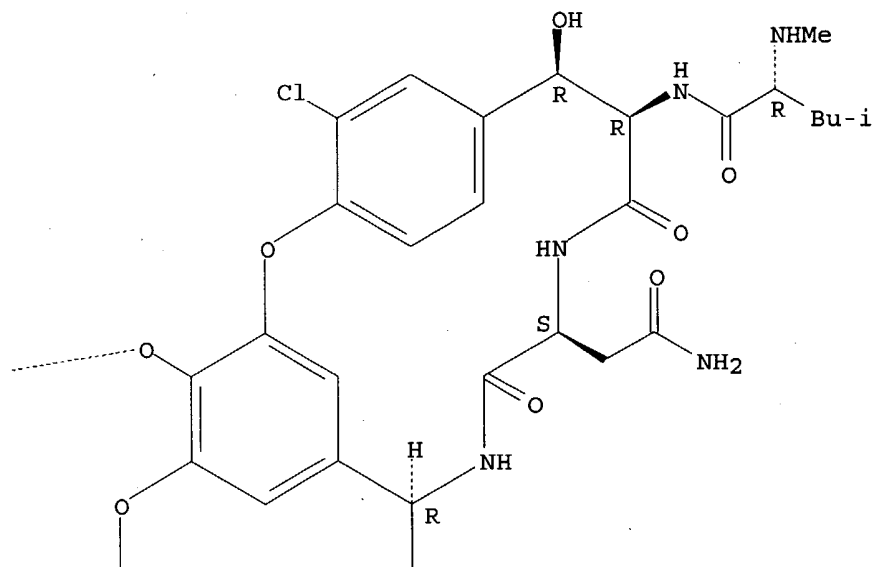
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Absolute stereochemistry.

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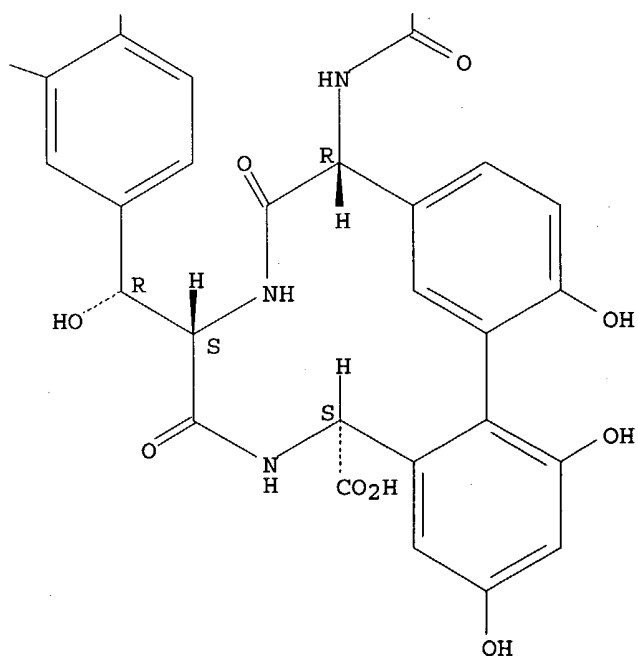
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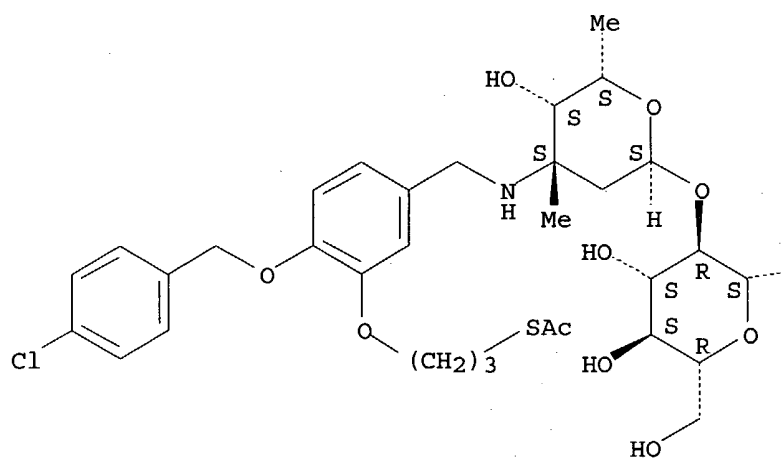


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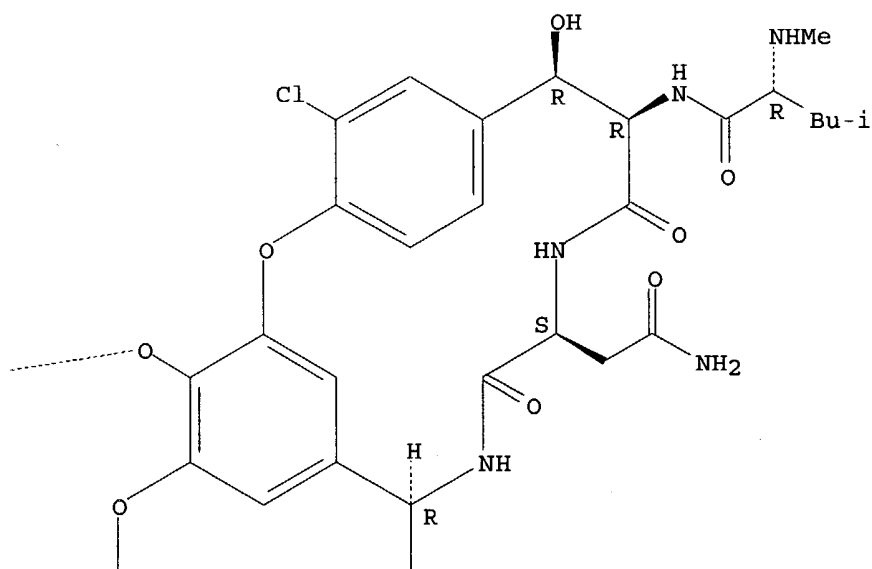
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CN	Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]-4-[(4-chlorophenyl)methoxy]phenyl]methyl]- (9CI)	(CA INDEX NAME)	

Absolute stereochemistry.

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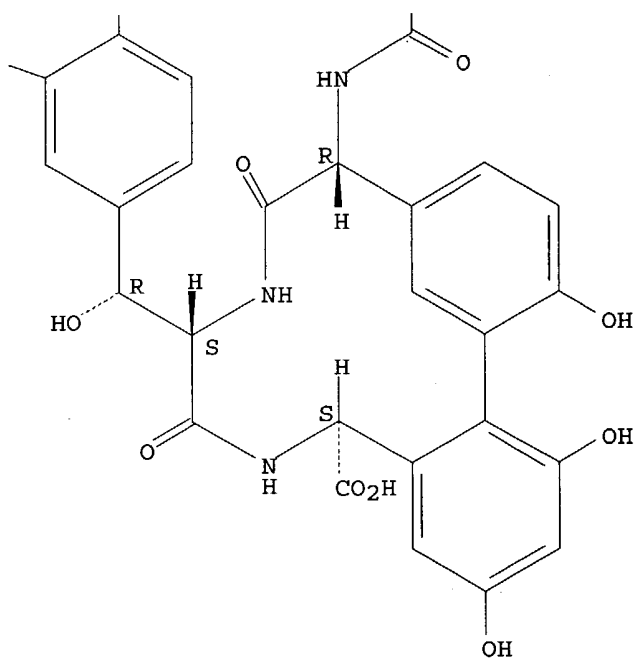
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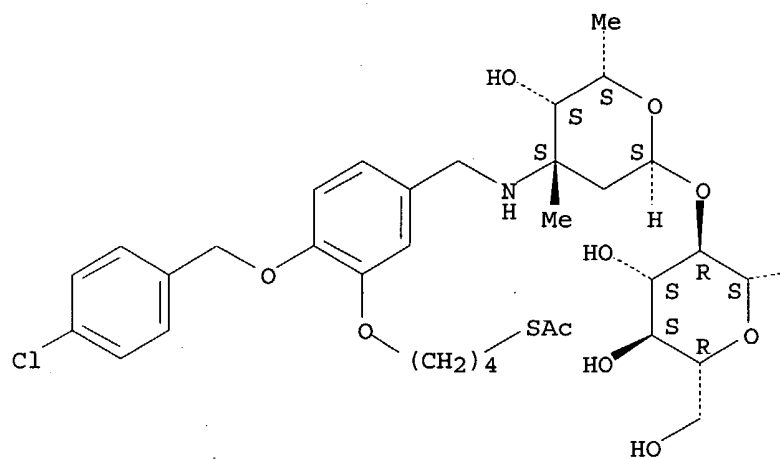


RN 383183-41-3 HCAPLUS

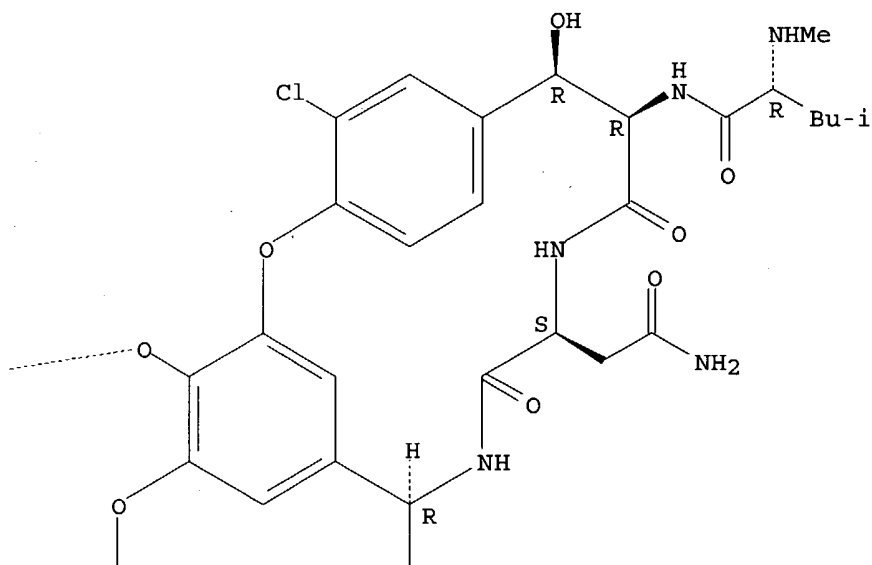
CN Vancomycin, N3' '-[[3-[4-(acetylthio)butoxy]-4-[(4-chlorophenyl)methoxy]phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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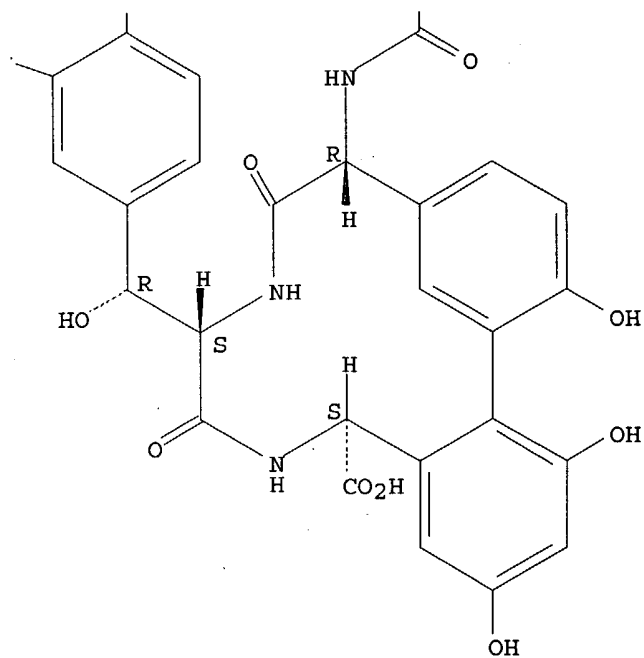
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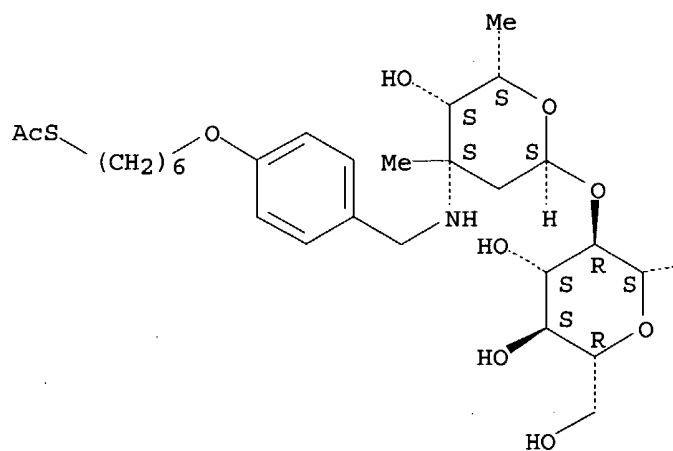


RN 383183-45-7 HCAPLUS

CN Vancomycin, N3'''-[[4-[[6-(acetylthio)hexyl]oxy]phenyl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

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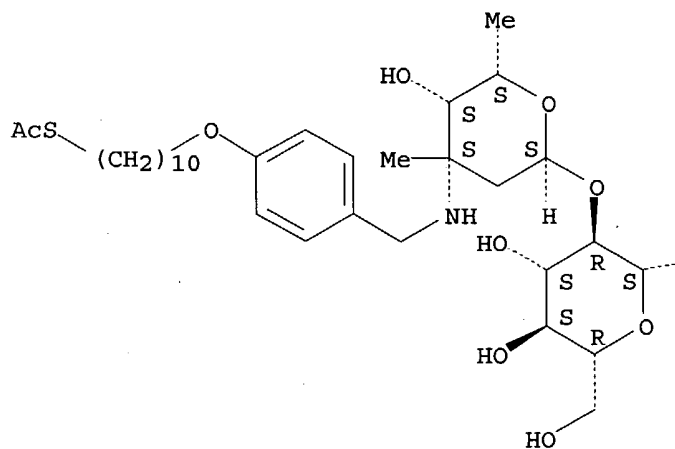


RN 383183-46-8 HCAPLUS

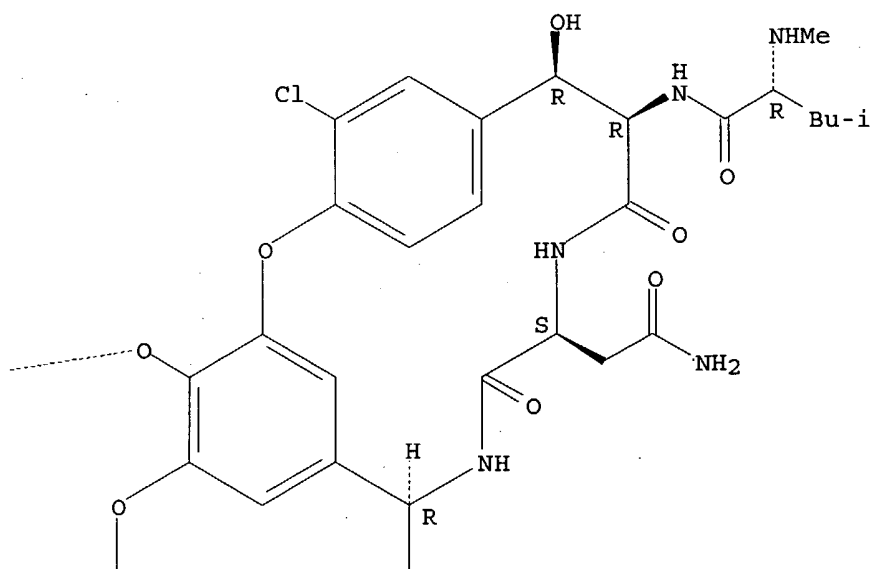
CN Vancomycin, N3'''-[[4-[[10-(acetylthio)decyloxy]phenyl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

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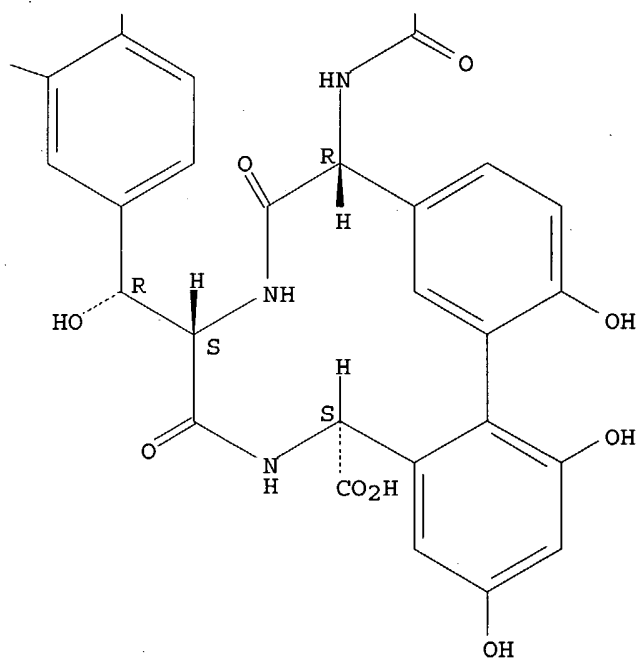
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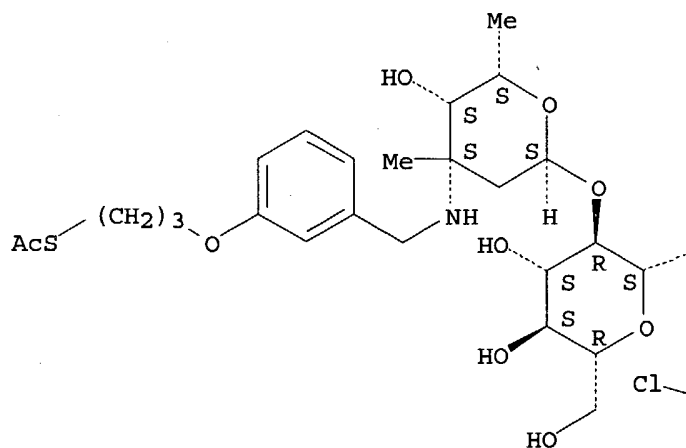


RN 383183-76-4 HCAPLUS

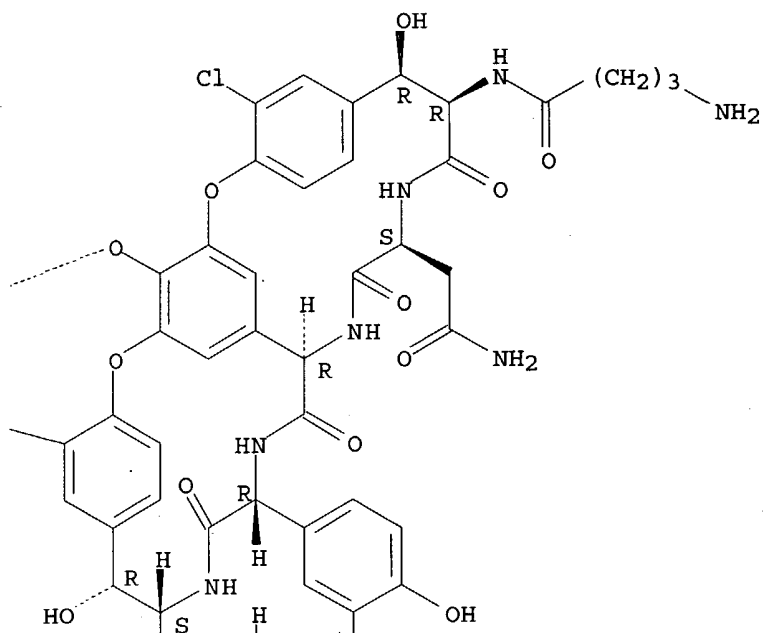
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-(4-amino-1-oxobutyl)-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

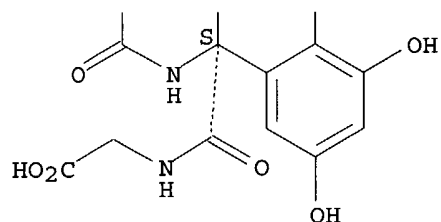
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IT 321362-17-8P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

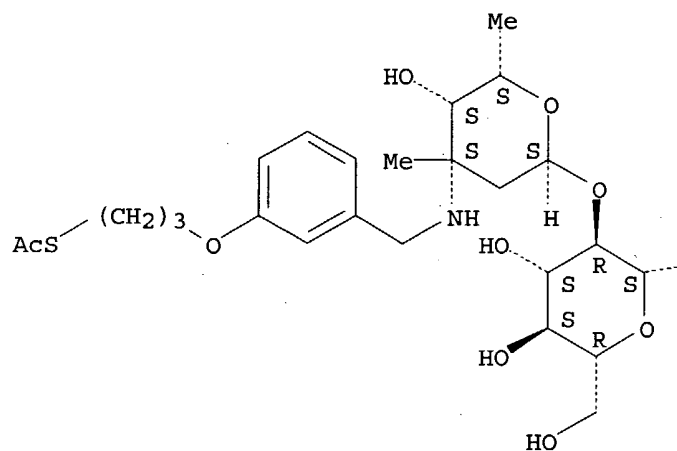
(synthesis of vancomycin and vancomycin analogs with activity against vancomycin-resistant bacteria)

RN 321362-17-8 HCAPLUS

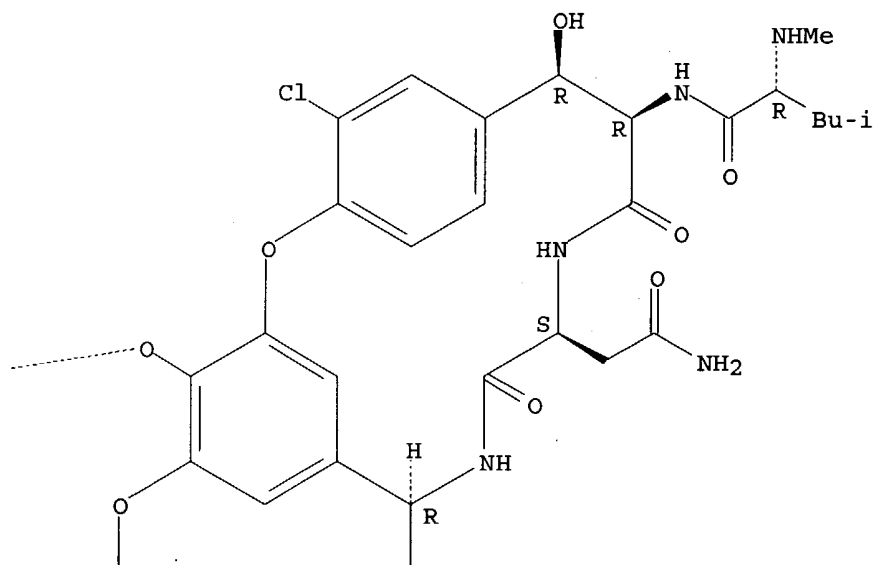
CN	Vancomycin, N3'''-[3-[3-(acetylthio)propoxy]phenyl]methyl]- (9CI)	(CA
	INDEX NAME)	

Absolute stereochemistry.

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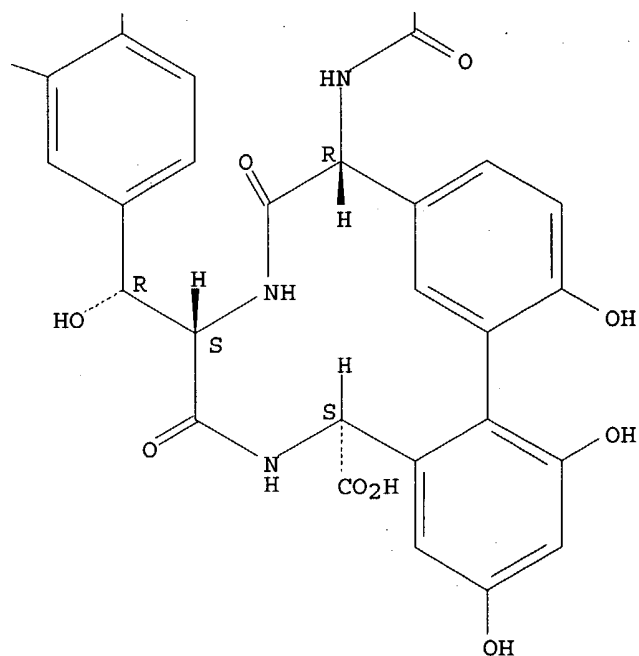
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IT 383183-42-4P 383183-43-5P 383183-44-6P
 383183-71-9P 383183-72-0P 383183-74-2P
 383183-75-3P 383183-78-6P 383183-79-7P
 383183-80-0P 383183-81-1P 383183-82-2P
 383184-95-0P 383184-97-2P 383184-99-4P
 383185-04-4P 383185-06-6P 383185-07-7P
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 383185-32-8P 383424-31-5P 383424-32-6P

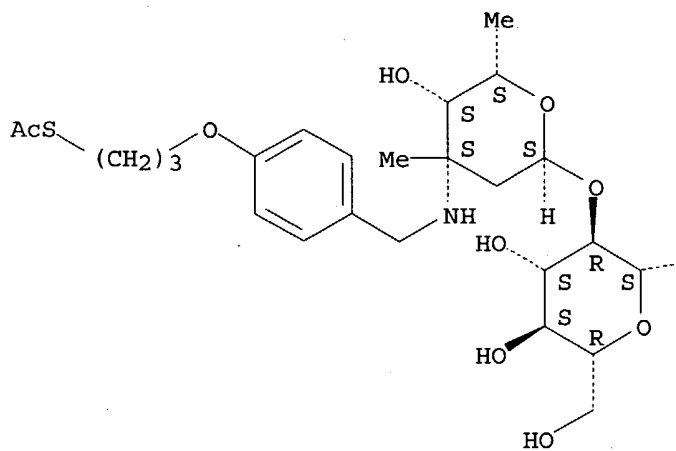
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation)
 (synthesis of vancomycin and vancomycin analogs with activity against
 vancomycin-resistant bacteria)

RN 383183-42-4 HCAPLUS

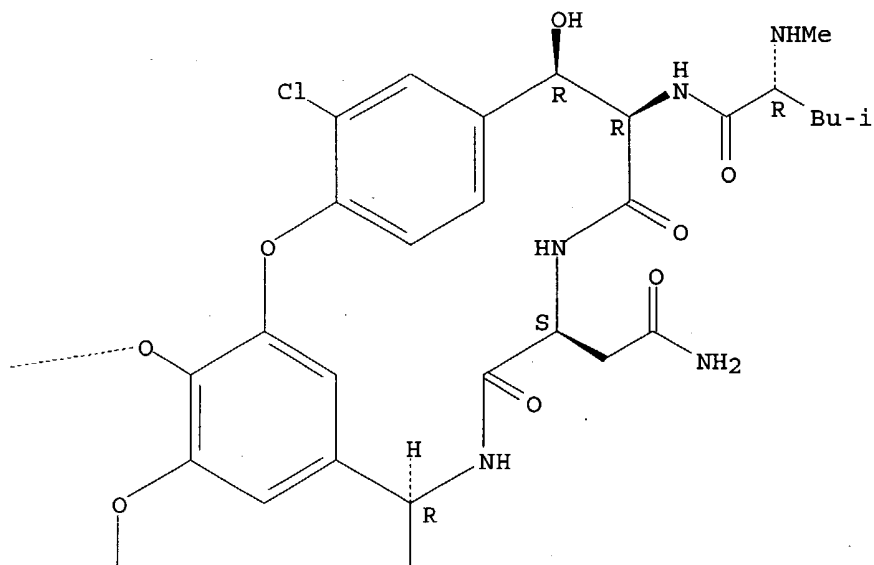
CN Vancomycin, N3'''-[[4-[3-(acetylthio)propoxy]phenyl]methyl]- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.

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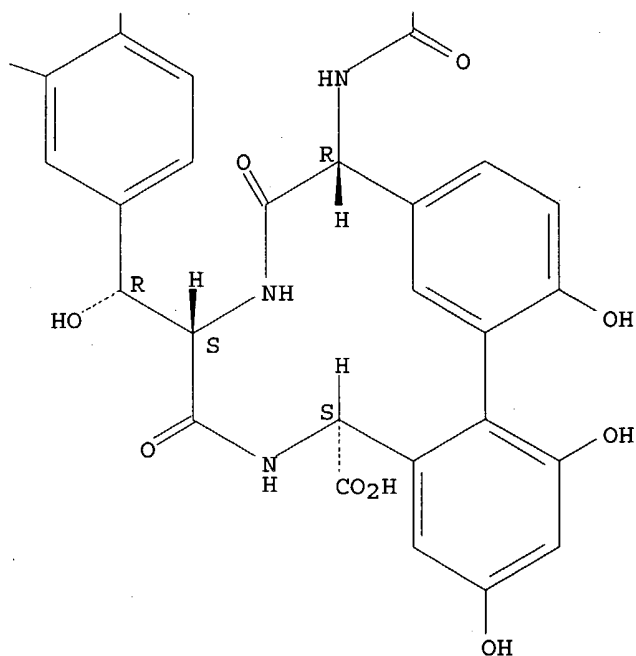
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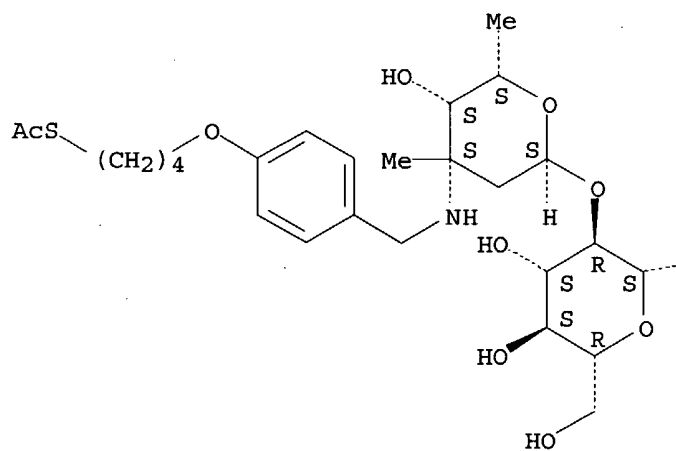


RN 383183-43-5 HCAPLUS

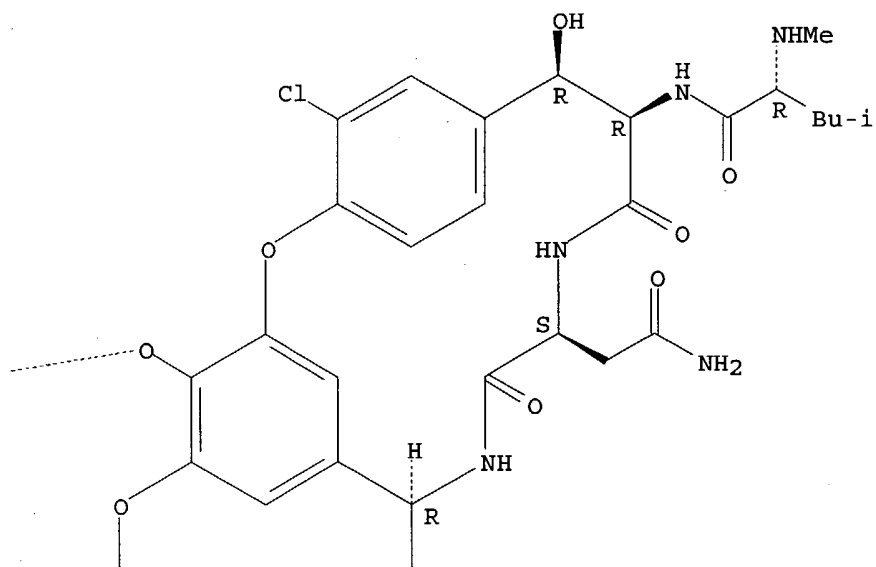
CN Vancomycin, N3'''-[[4-[4-(acetylthio)butoxy]phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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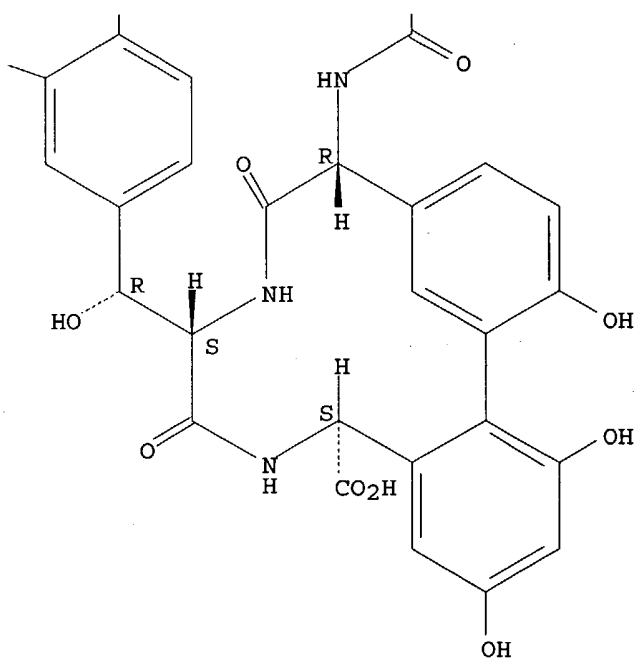
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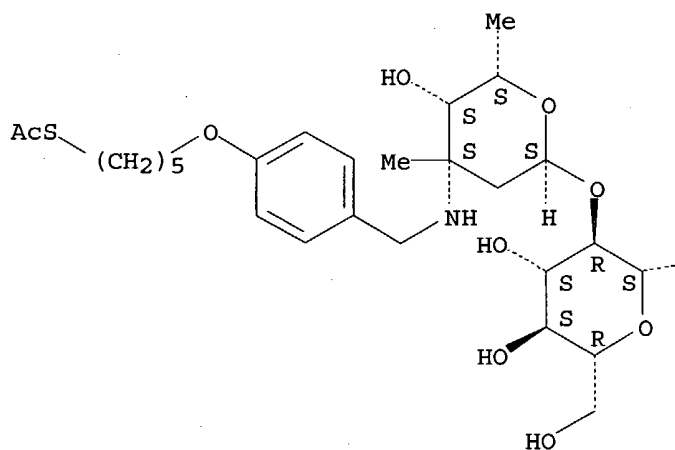


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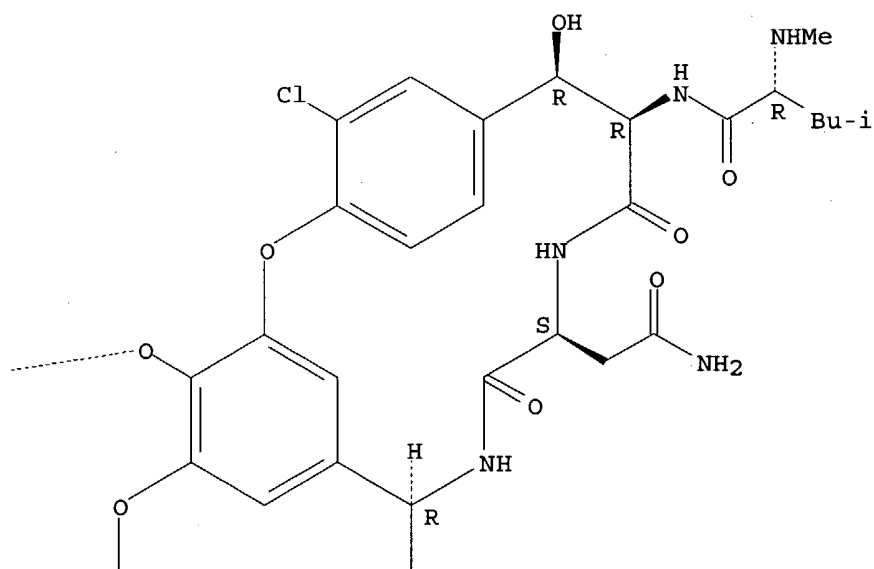
CN Vancomycin, N3'''-[[4-[[5-(acetylthio)pentyl]oxy]phenyl]methyl] - (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

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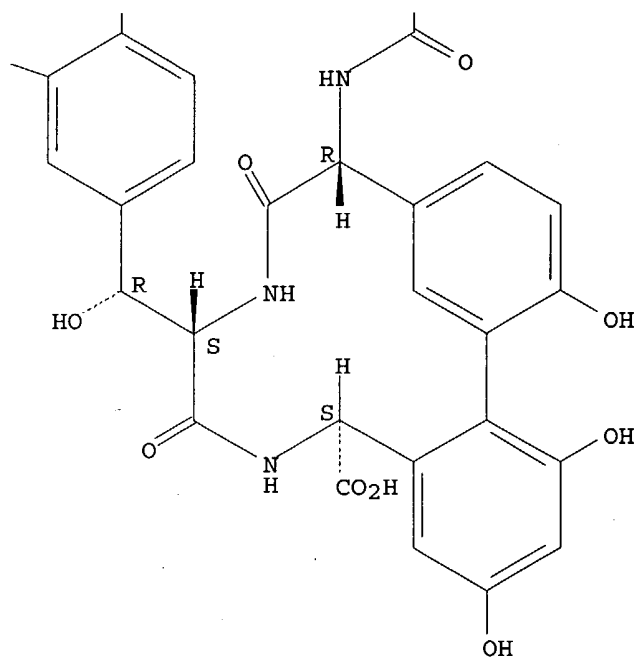
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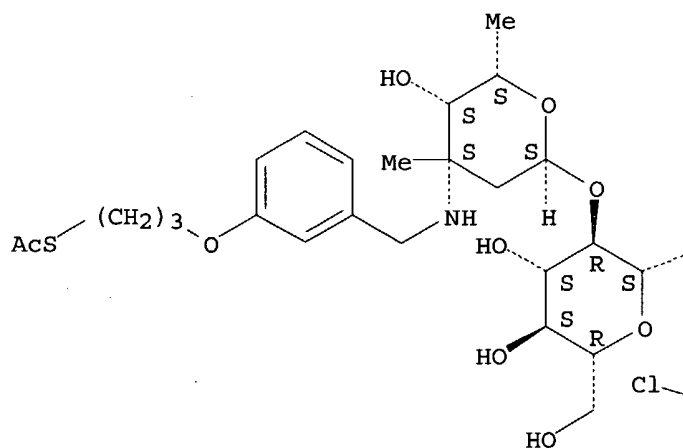


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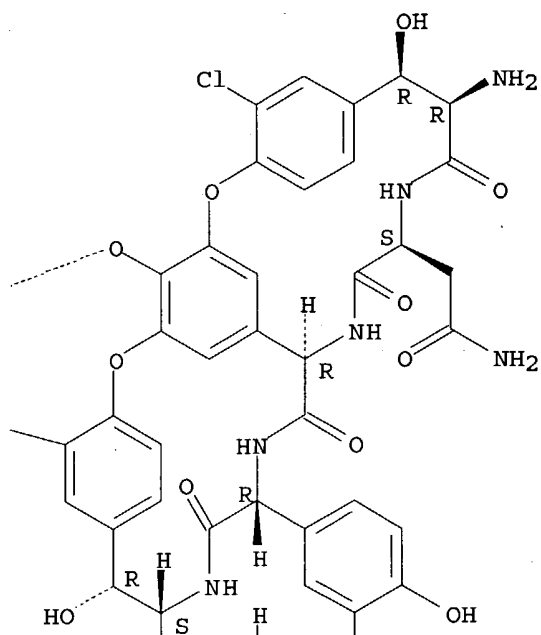
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-28-
 [[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-
 (methylamino)-1-oxopentyl]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

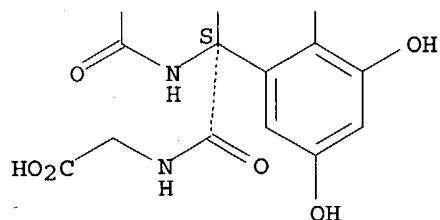
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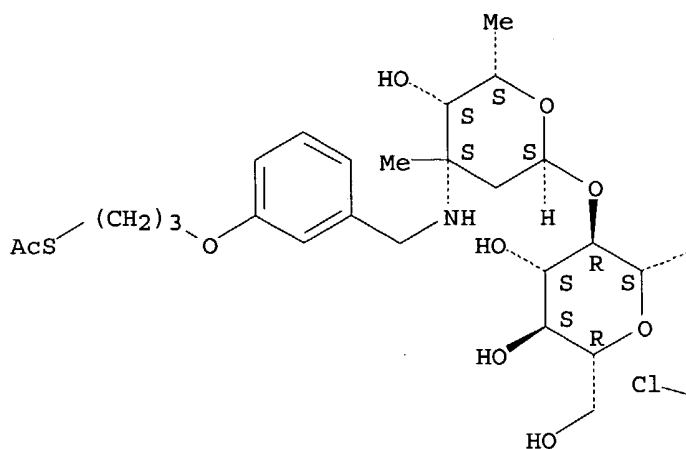


RN 383183-72-0 HCAPLUS

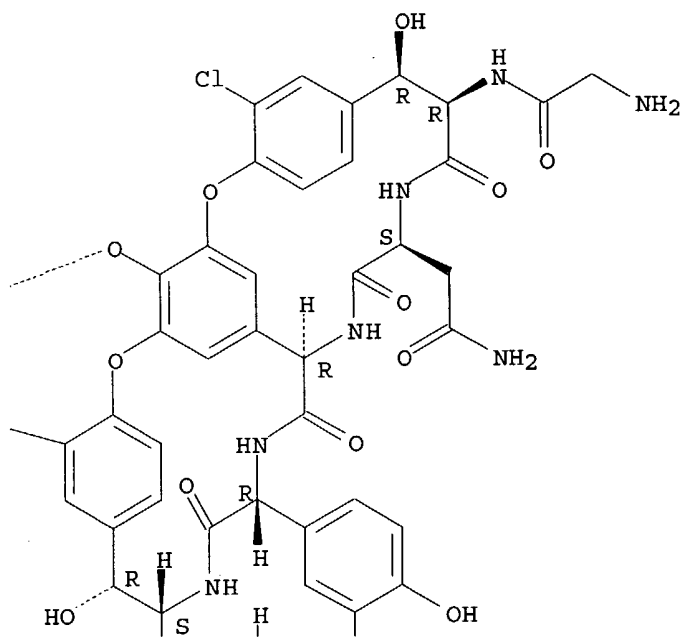
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-(aminoacetyl)-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

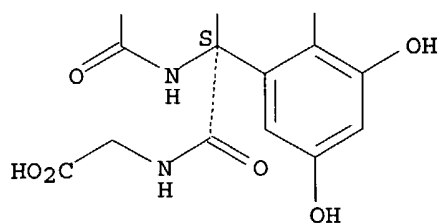
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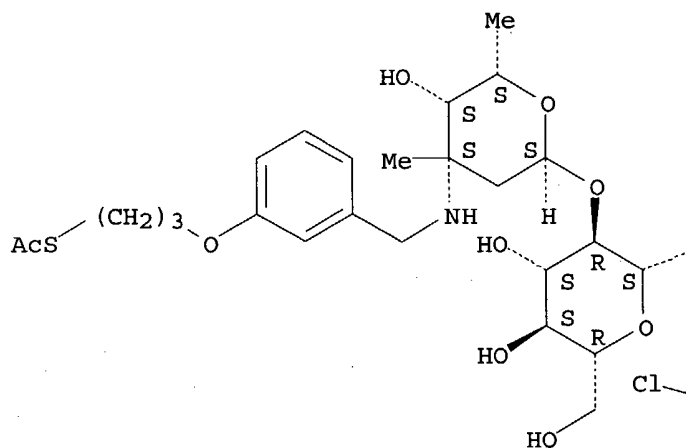


RN 383183-74-2 HCAPLUS

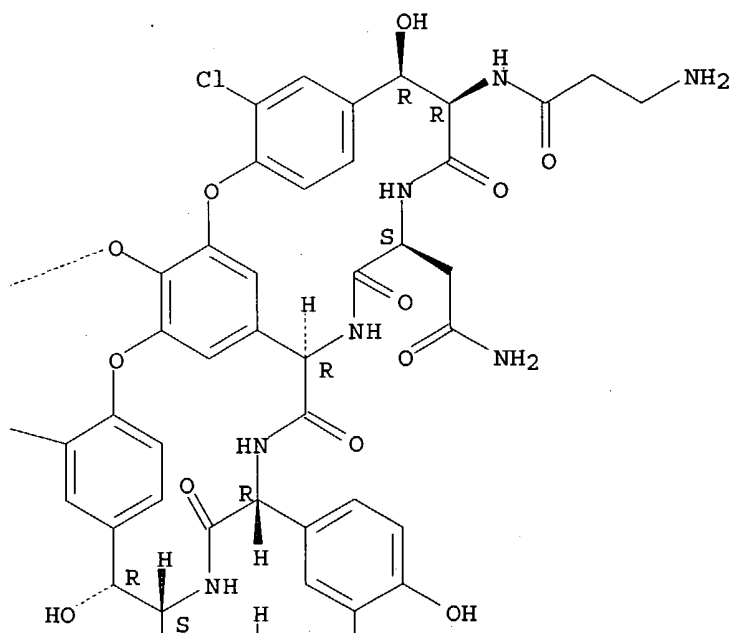
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-(3-amino-1-oxopropyl)-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

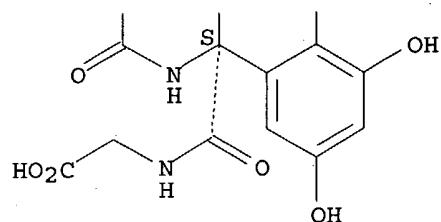
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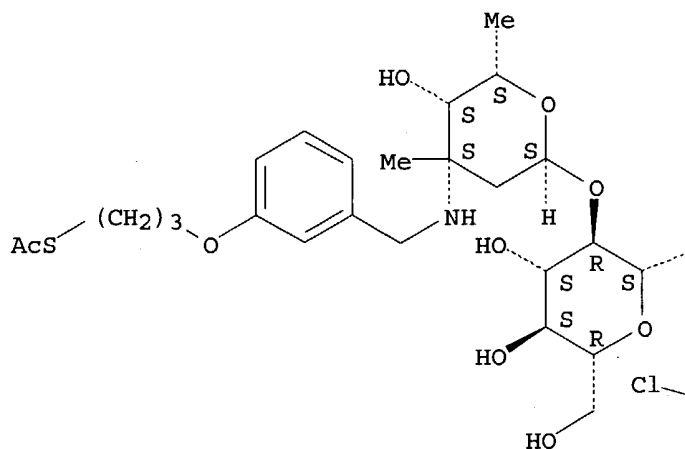


RN 383183-75-3 HCAPLUS

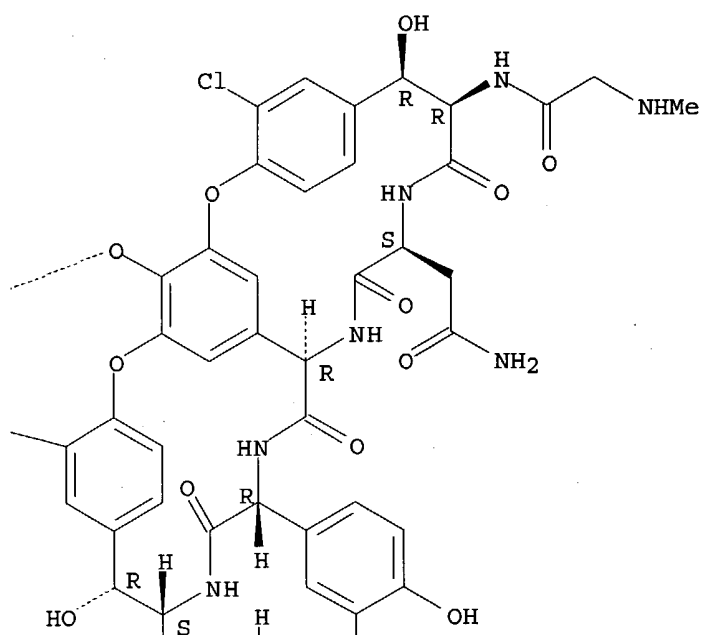
CN Vancomycin, N3''' - [[3-[3-(acetylthio)propoxy]phenyl]methyl]-28-
 [[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-
 (methylamino)-1-oxopentyl]-49-[(methylamino)acetyl]- (9CI) (CA INDEX
 NAME)

Absolute stereochemistry.

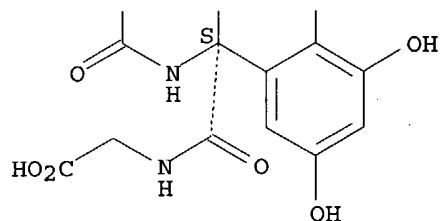
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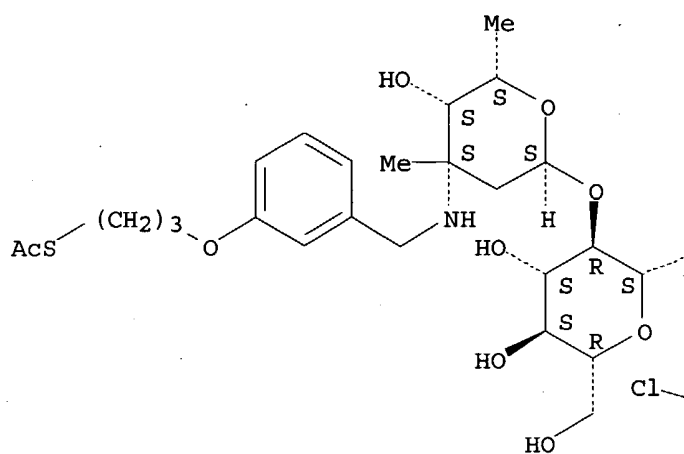


RN 383183-78-6 HCAPLUS

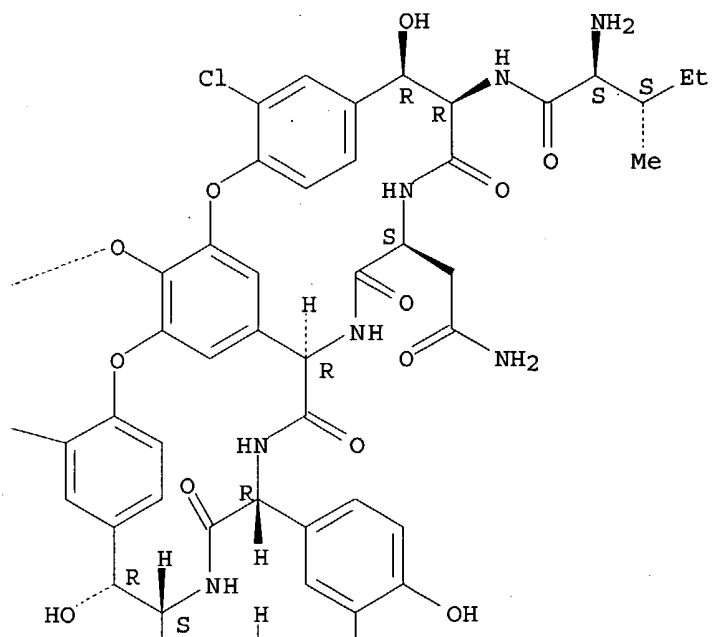
CN Vancomycin, N3'''-[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S,3S)-2-amino-3-methyl-1-oxopentyl]-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

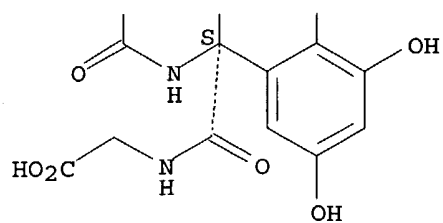
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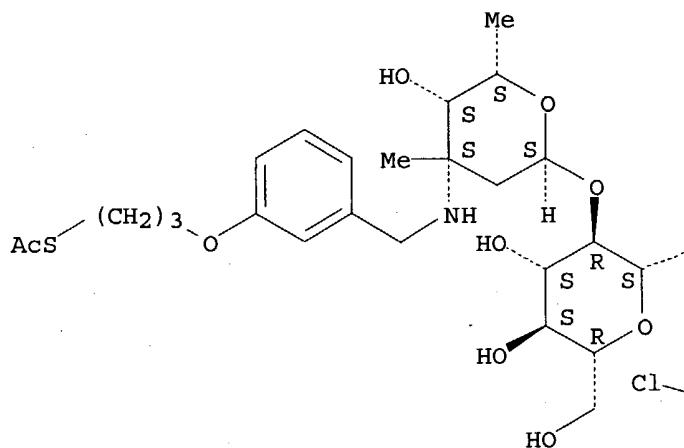
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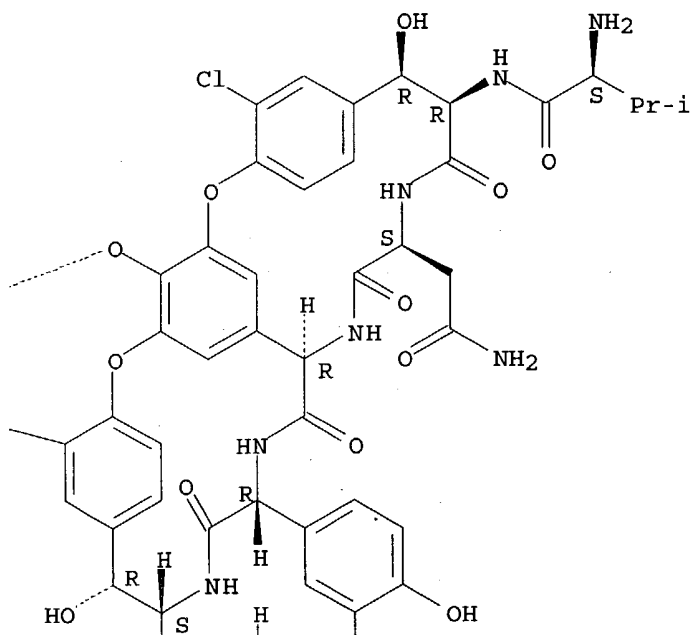
RN 383183-79-7 HCAPLUS
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-3-methyl-1-oxobutyl]-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

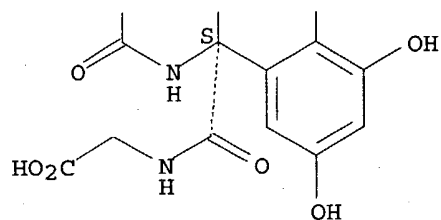
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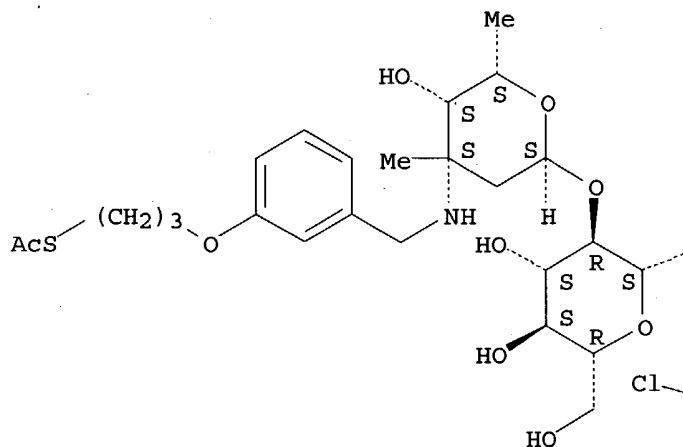


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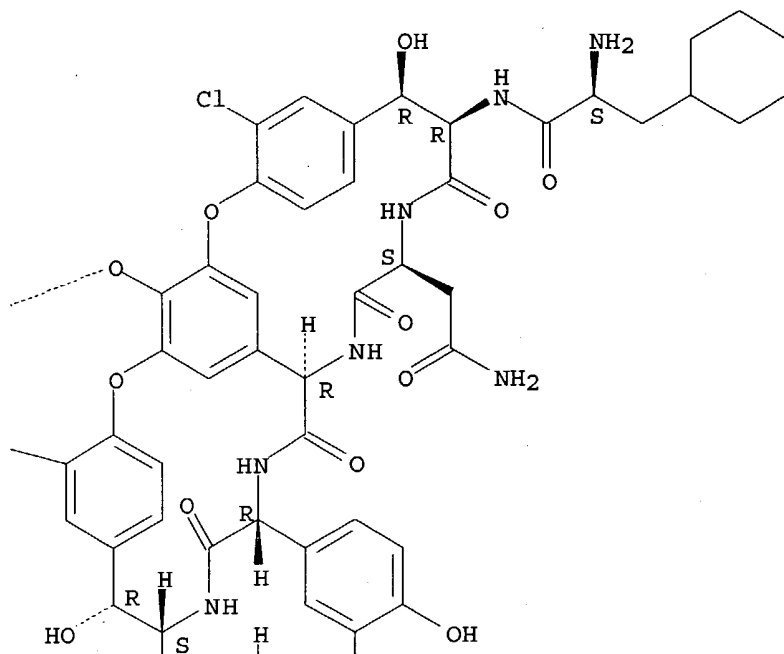
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-3-cyclohexyl-1-oxopropyl]-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

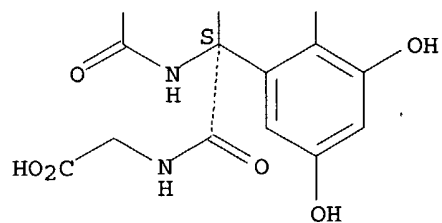
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RN 383183-81-1 HCAPLUS

CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-28-
 [[[(carboxymethyl)amino]carbonyl]-28-decarboxy-56-demethyl-, (51S) - (9CI)
 (CA INDEX NAME)

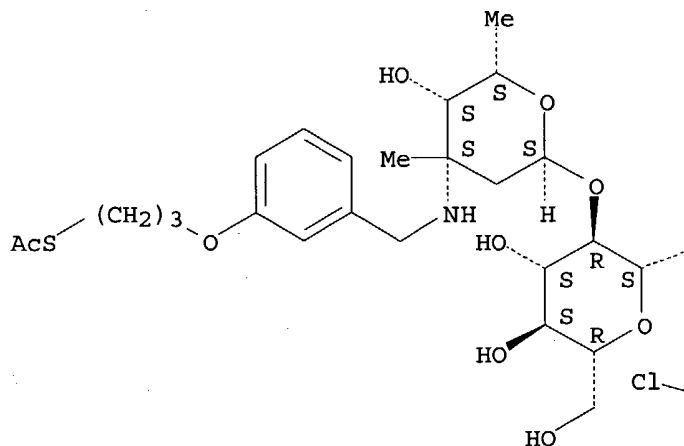
Absolute stereochemistry.

RN 383183-82-2 HCAPLUS

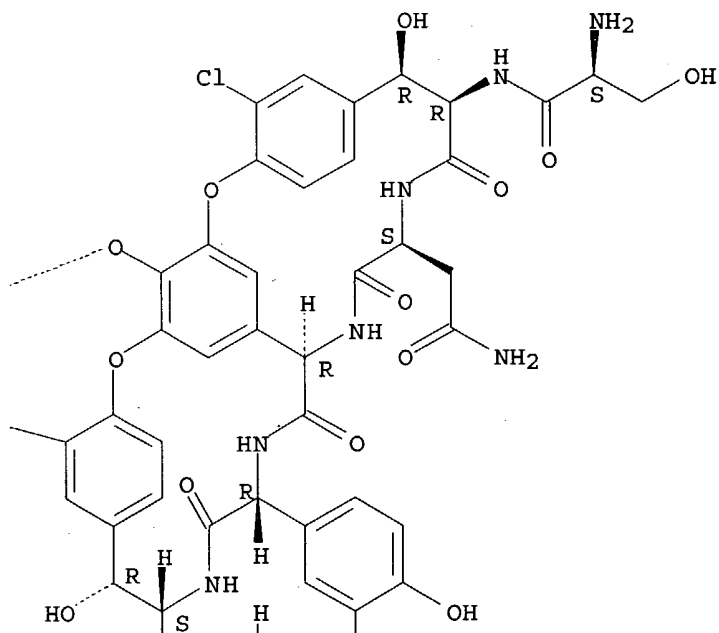
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-3-hydroxy-1-oxopropyl]-28-[[[(carboxymethyl)amino]carbonyl]-28-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

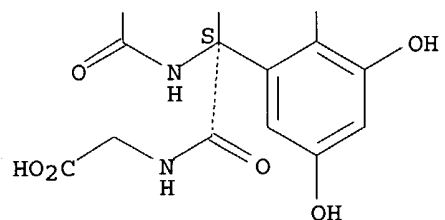
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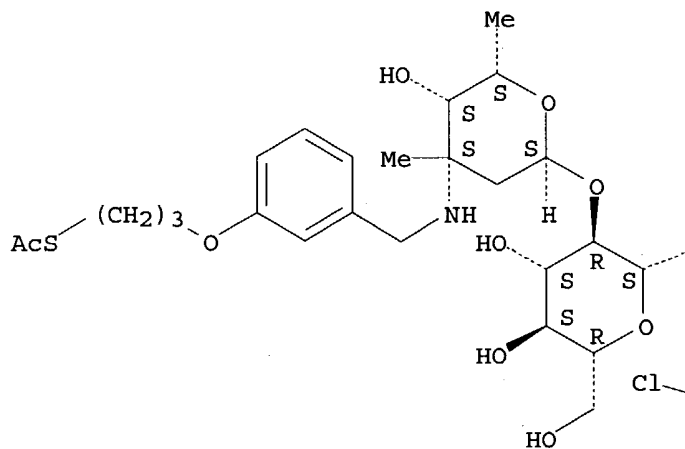


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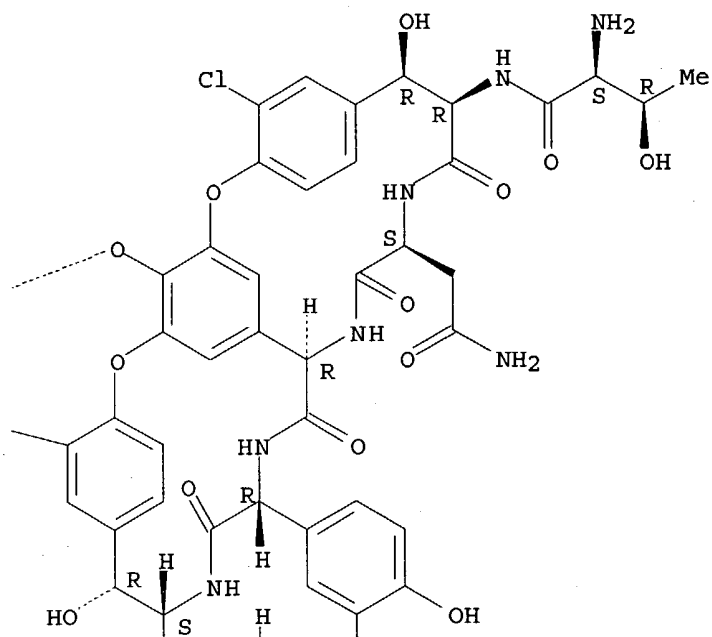
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S,3R)-2-amino-3-hydroxy-1-oxobutyl]-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

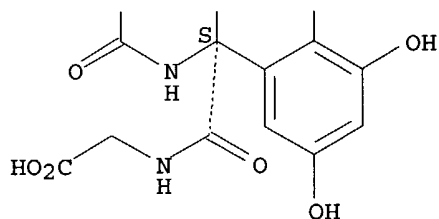
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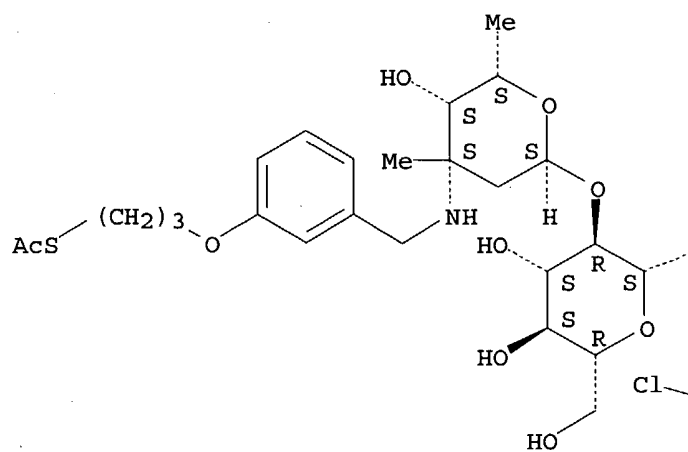


RN 383184-97-2 HCAPLUS

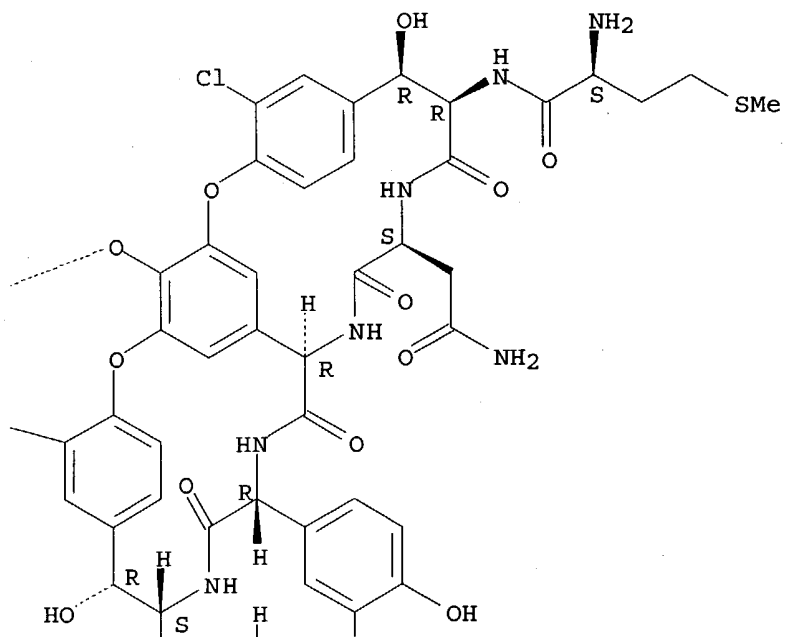
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-4-(methylthio)-1-oxobutyl]-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

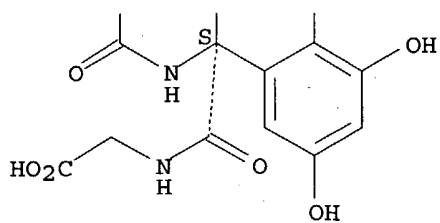
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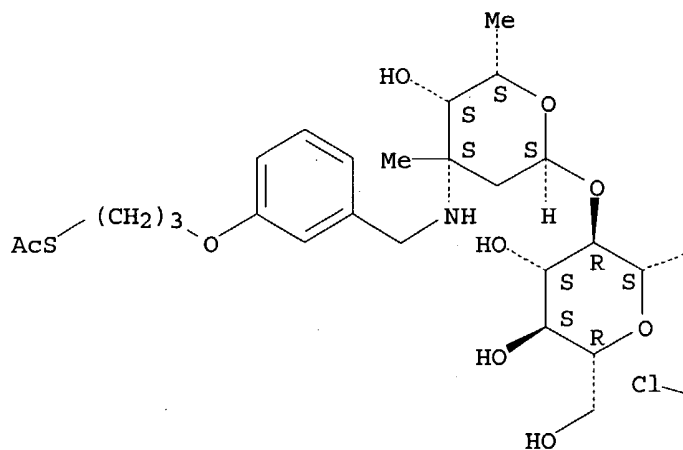


RN 383184-99-4 HCAPLUS

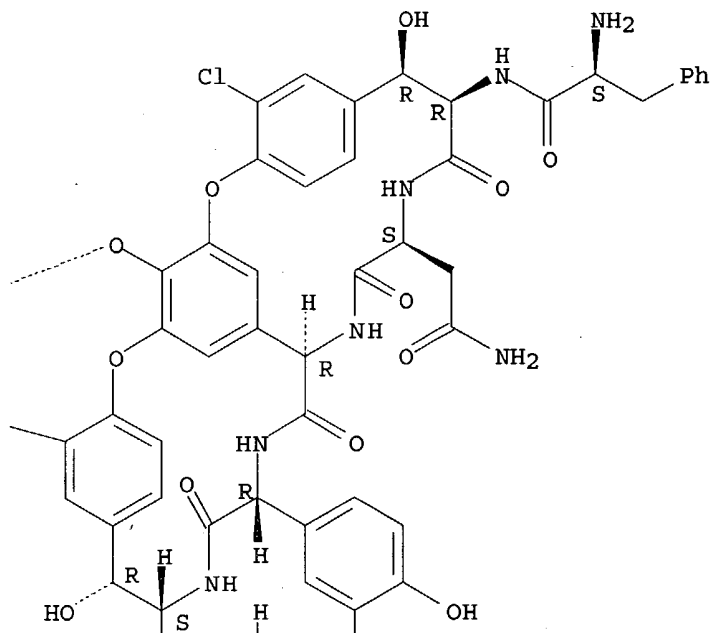
Vancomycin, N3''' - [[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-1-oxo-3-phenylpropyl]-26-[[(carboxymethyl) amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

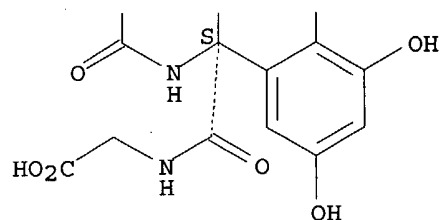
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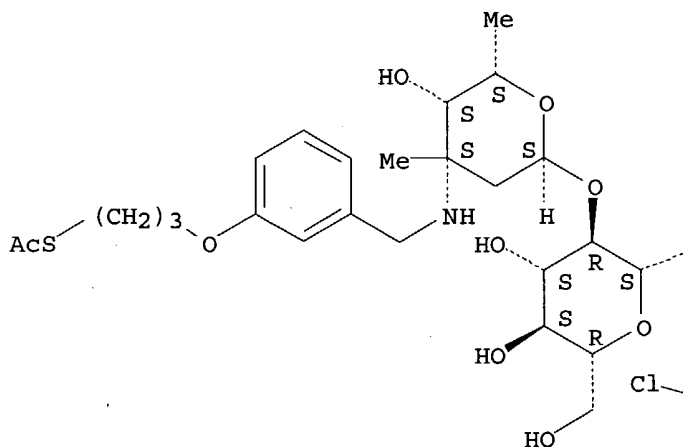


RN 383185-04-4 HCAPLUS

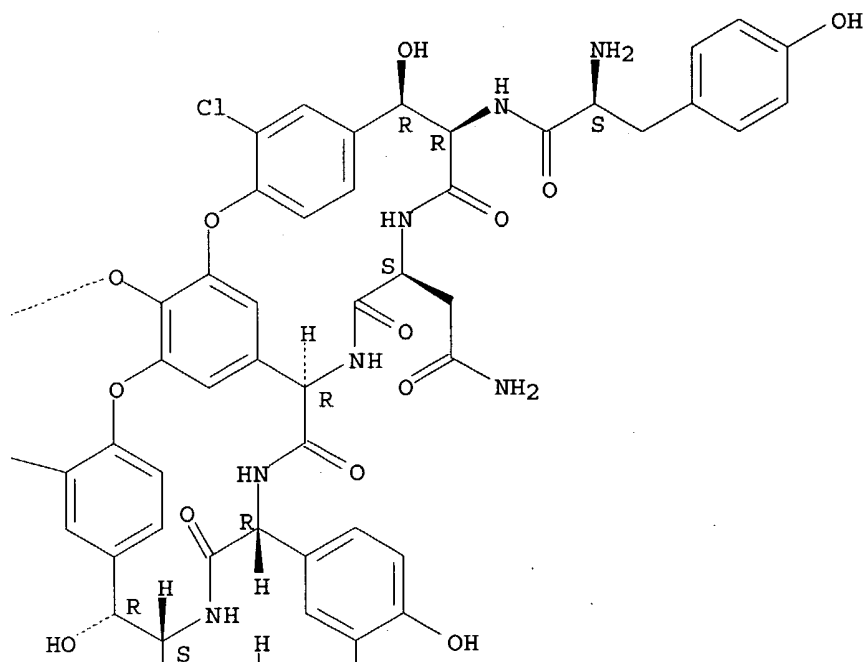
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-3-(4-hydroxyphenyl)-1-oxopropyl]-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

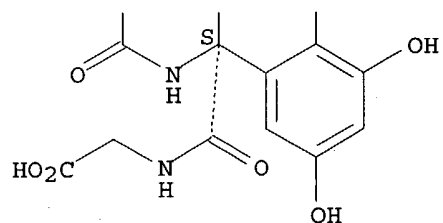
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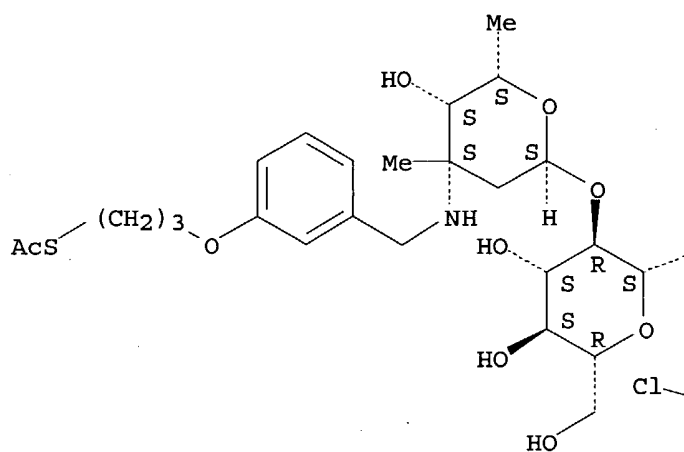


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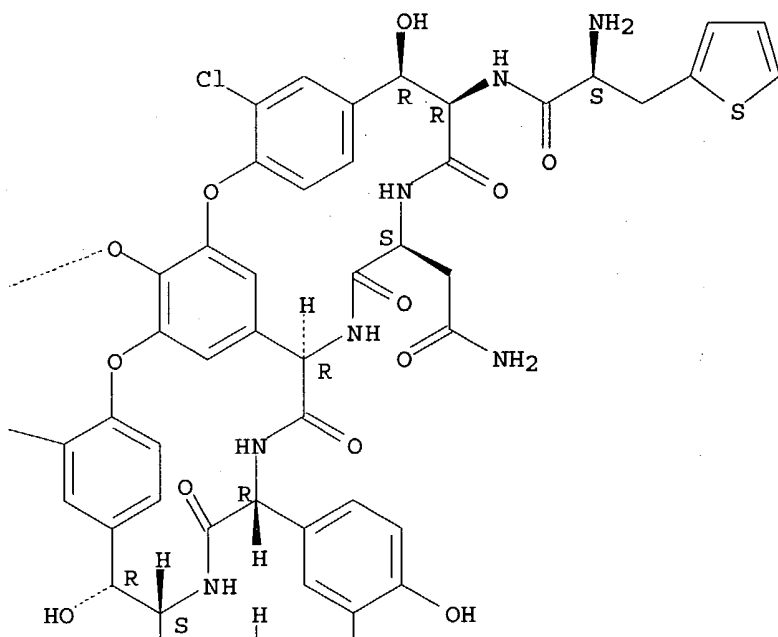
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-1-oxo-3-(2-thienyl)propyl]-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

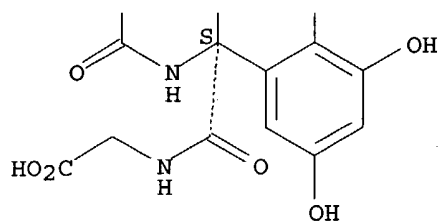
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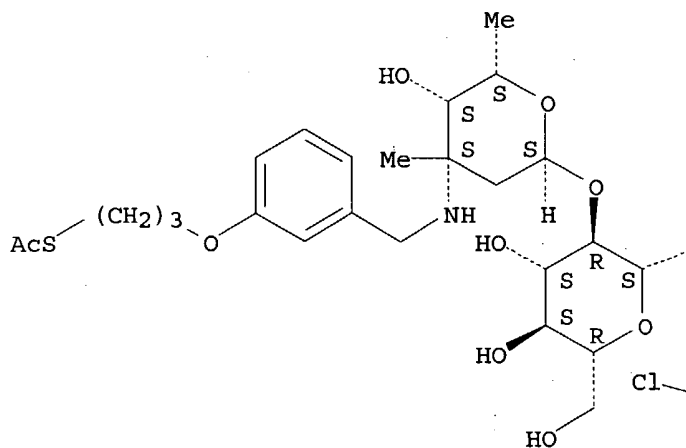
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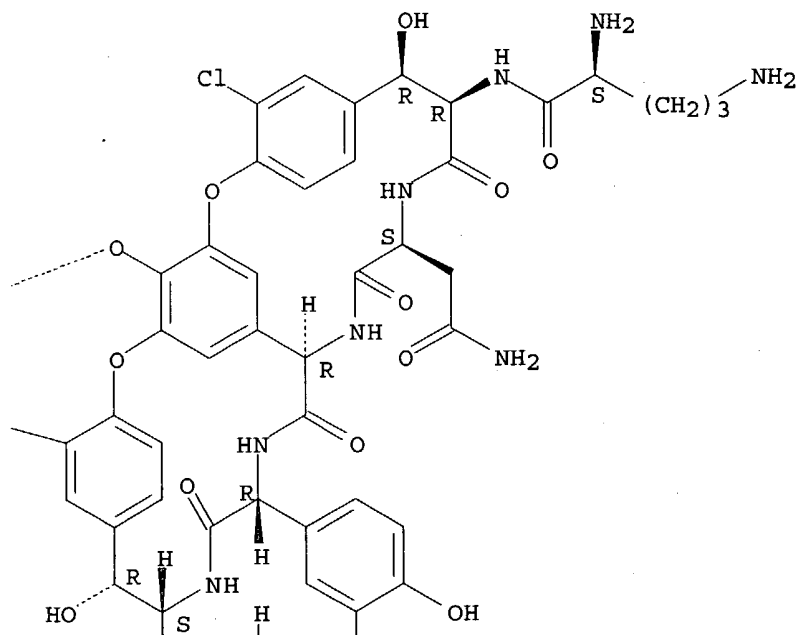
RN 383185-07-7 HCAPLUS
 CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-54-amino-26-
 [[(carboxymethyl)amino]carbonyl]-26-decarboxy-53,56-didemethyl- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.

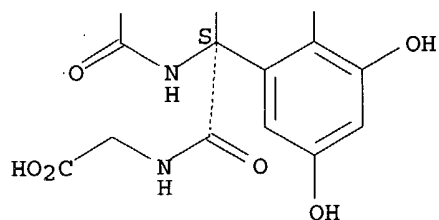
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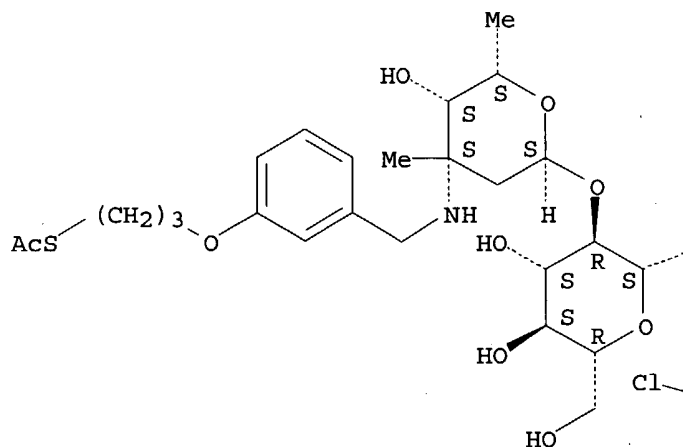


RN 383185-09-9 HCAPLUS

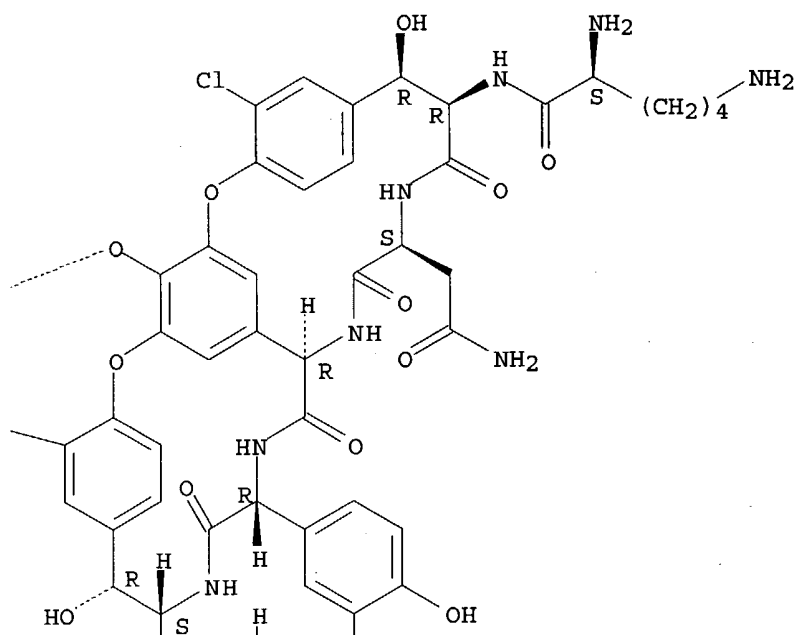
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 [[[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-
 (methylamino)-1-oxopentyl]-49-[(2S)-2,6-diamino-1-oxohexyl]- (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.

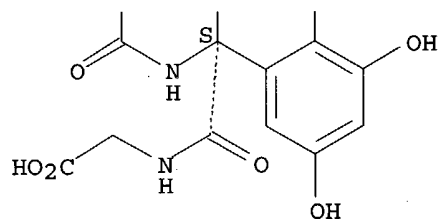
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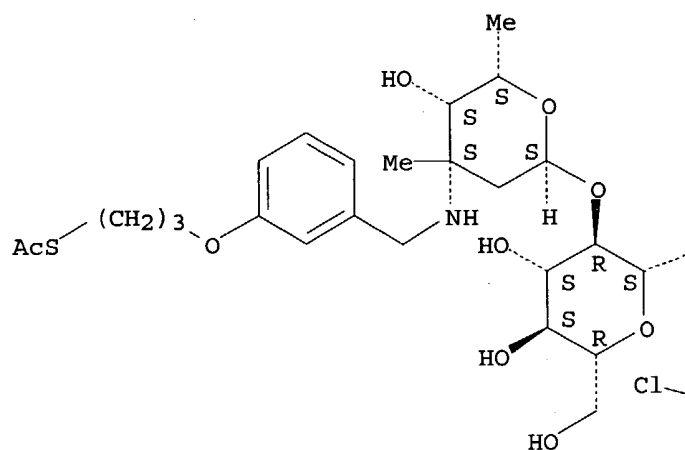


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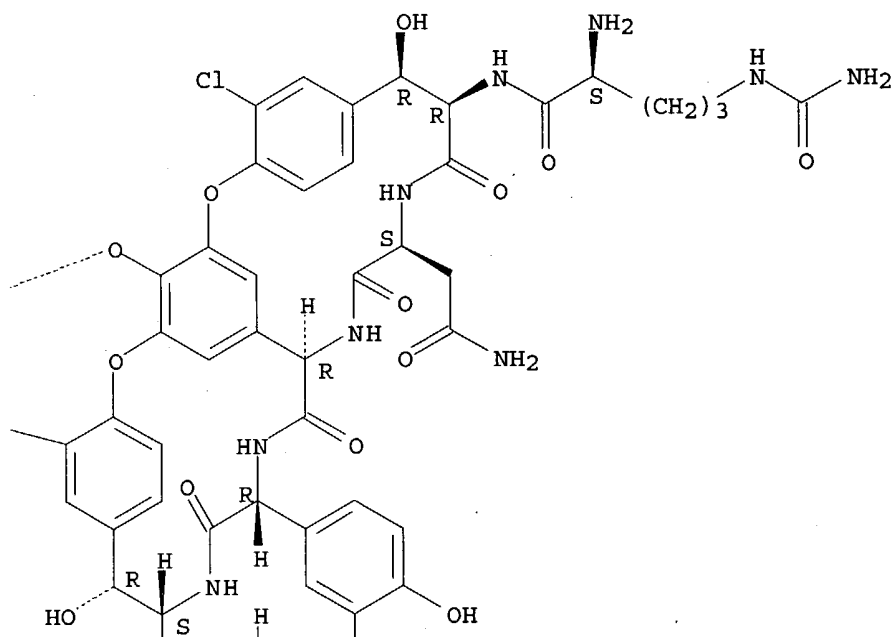
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-54-
 [(aminocarbonyl)amino]-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-
 53,56-didemethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

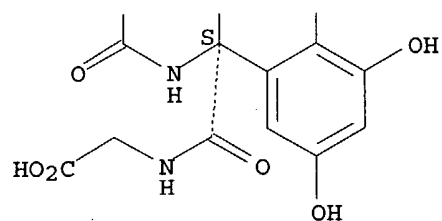
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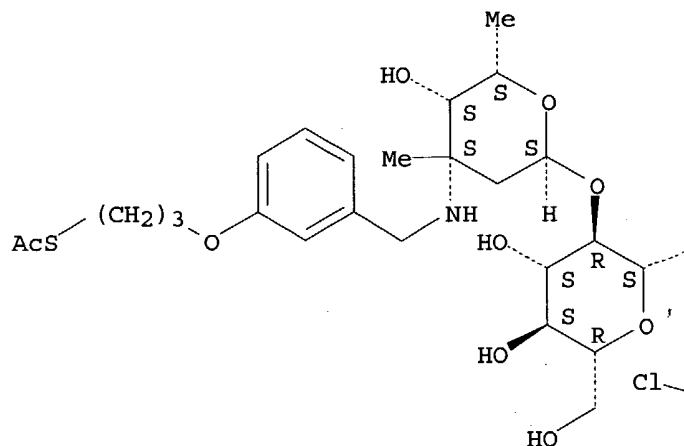
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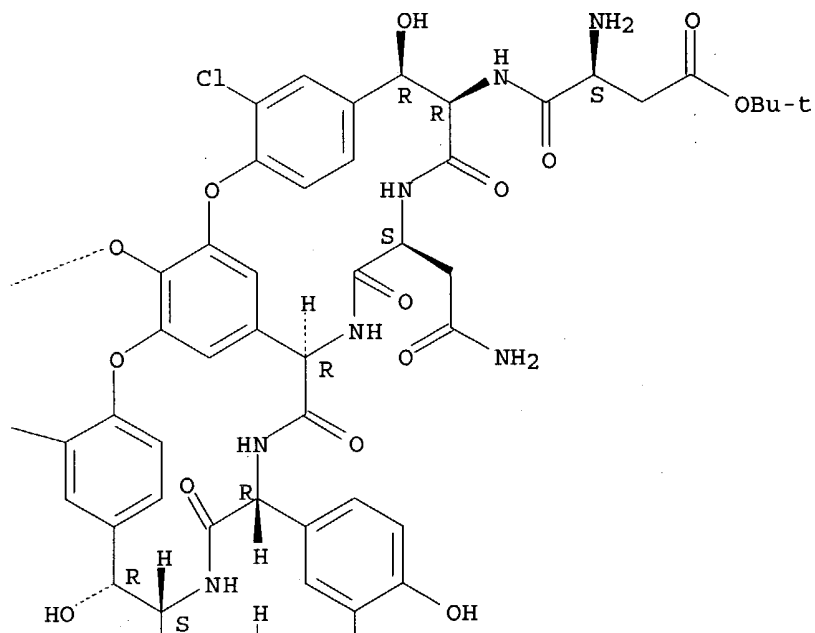
RN 383185-12-4 HCAPLUS
CN Vancomycin, N3''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-4-(1,1-dimethylethoxy)-1,4-dioxobutyl]-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

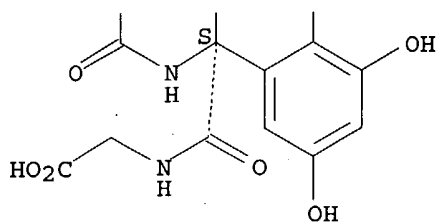
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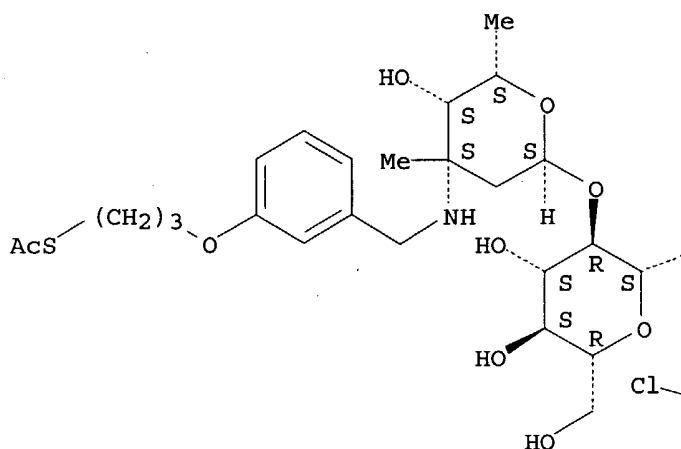


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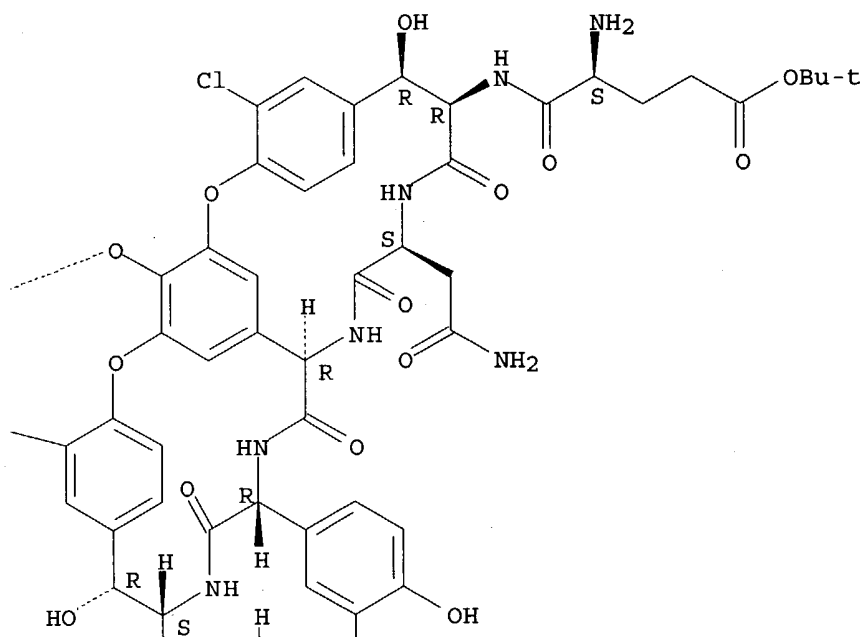
CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-54-(1,1-dimethylethoxy)-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-53,56-didemethyl-54-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

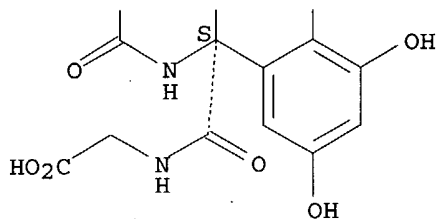
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RN 383424-31-5 HCAPLUS

CN Vancomycin, N3'''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-[(2S)-2-amino-1-oxopropyl]-26-[[[(carboxymethyl)amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

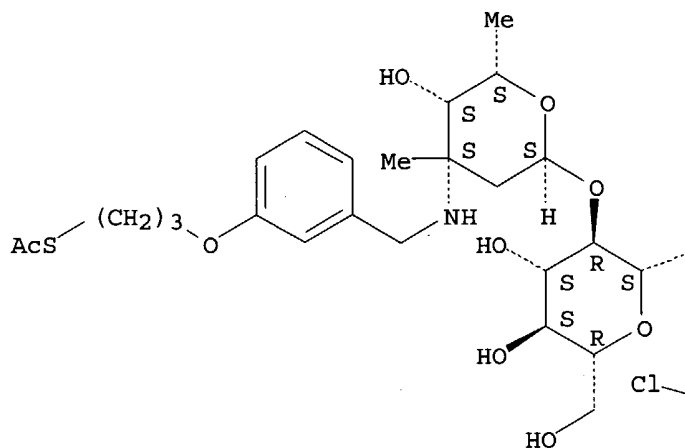
Absolute stereochemistry.

RN 383424-32-6 HCAPLUS

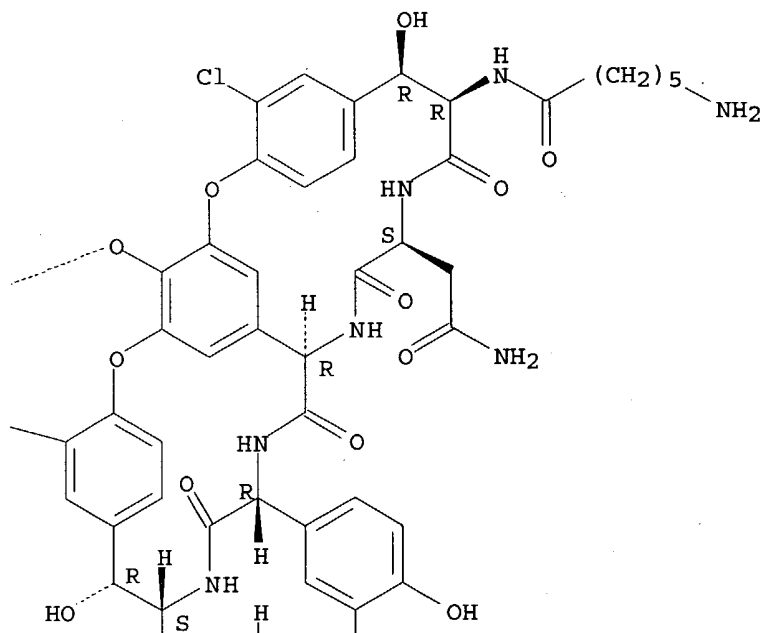
CN Vancomycin, N3'''-[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-(6-amino-1-oxohexyl)-26-[[[carboxymethyl]amino]carbonyl]-26-decarboxy-49-de[4-methyl-2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

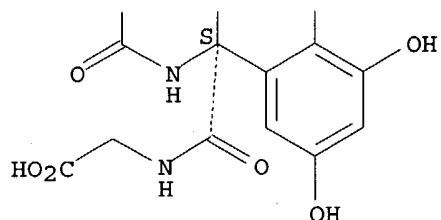
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IT 383424-29-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

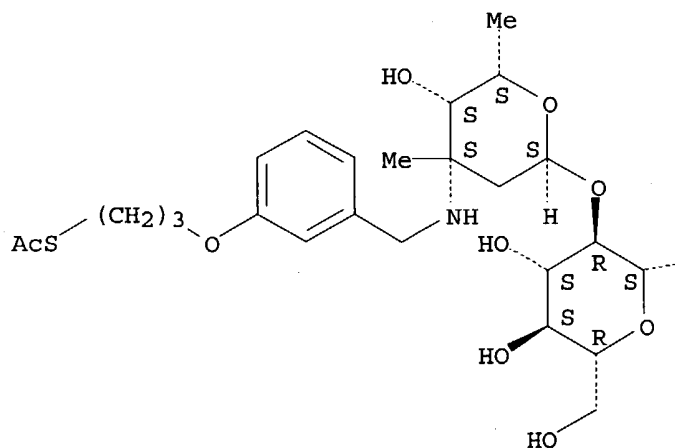
(synthesis of vancomycin and vancomycin analogs with activity against vancomycin-resistant bacteria)

RN 383424-29-1 HCAPLUS

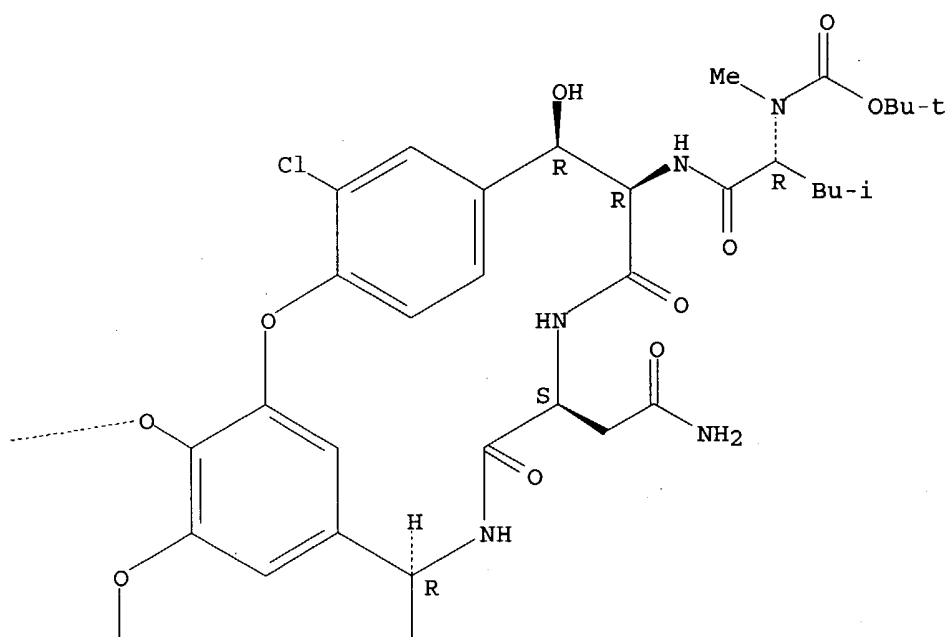
Vancomycin, N3'''-[3-[3-(acetylthio)propoxy]phenyl]methyl]-56-[(1,1-dimethylethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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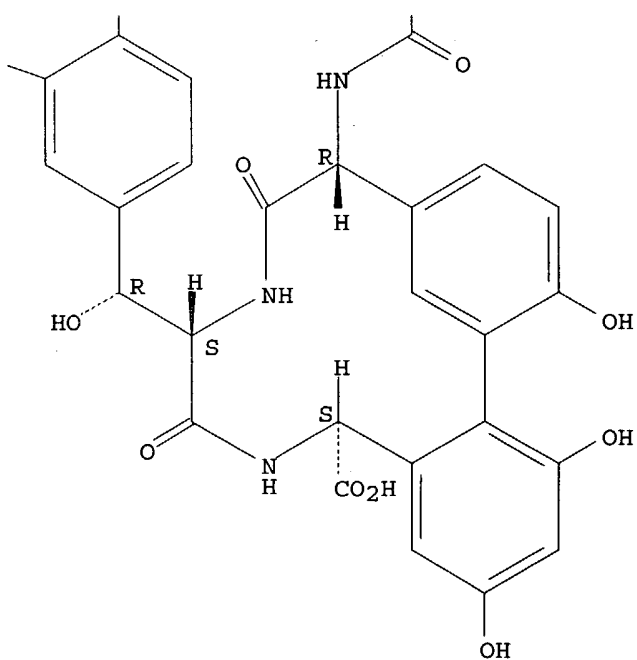
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IT 383424-30-4P

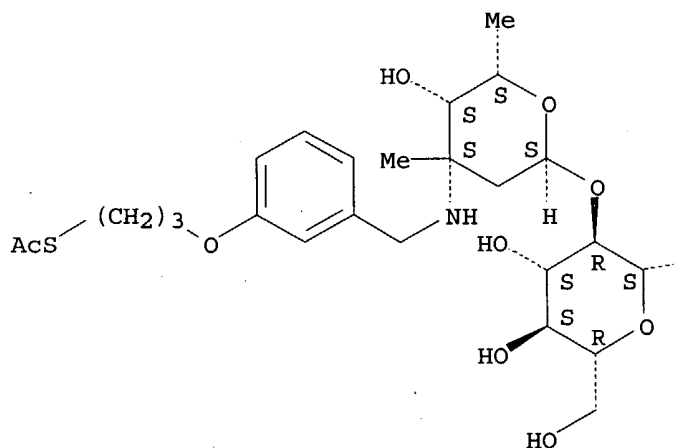
RL: SPN (Synthetic preparation); PREP (Preparation)
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vancomycin-resistant bacteria)

RN 383424-30-4 HCAPLUS

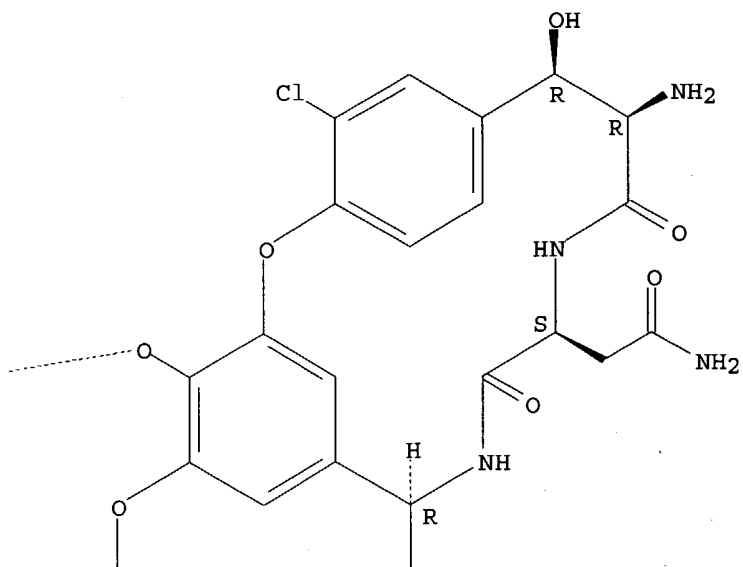
CN Vancomycin, N3''-[[3-[3-(acetylthio)propoxy]phenyl]methyl]-49-de[4-methyl-
2-(methylamino)-1-oxopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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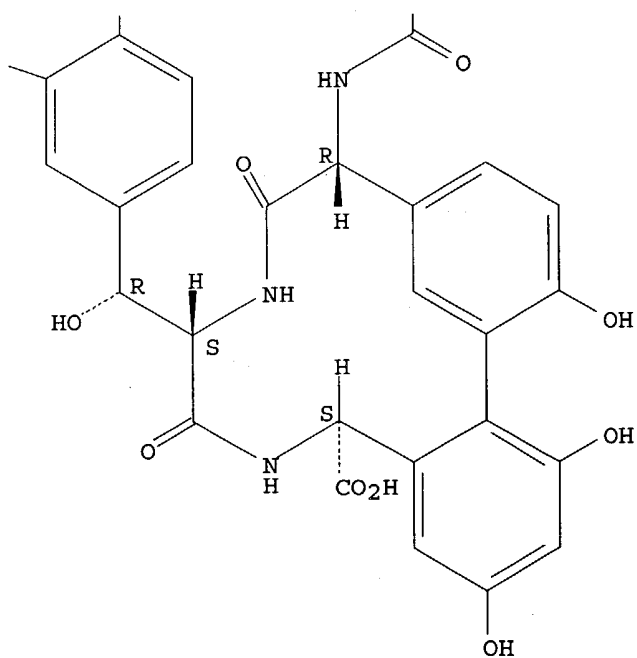
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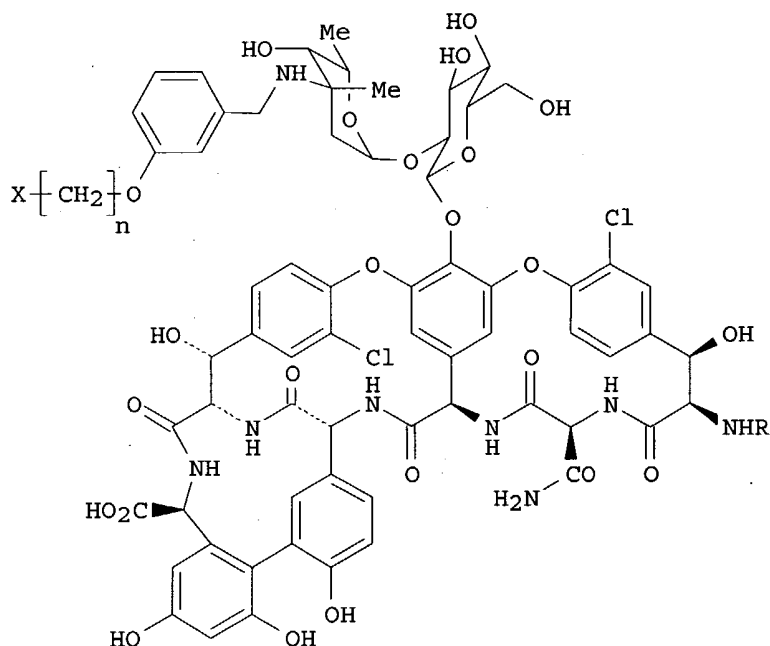
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L65 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN
 AN 2000:818978 HCAPLUS
 DN 134:116215
 ED Entered STN: 22 Nov 2000
 TI Target-accelerated combinatorial synthesis and discovery of highly potent antibiotics effective against vancomycin-resistant bacteria
 AU Nicolaou, K. C.; Hughes, Robert; Cho, Suk Young; Winssinger, Nicolas; Smethurst, Christian; Labischinski, Harald; Endermann, Rainer
 CS Skaggs Inst. Chemical Biology, Scripps Res. Inst., La Jolla, CA, 92037, USA
 SO Angewandte Chemie, International Edition (2000), 39(21), 3823-3828
 CODEN: ACIEF5; ISSN: 1433-7851
 PB Wiley-VCH Verlag GmbH
 DT Journal
 LA English
 CC 34-3 (Amino Acids, Peptides, and Proteins)
 Section cross-reference(s): 1
 OS CASREACT 134:116215
 GI

↓
 Oct 2000



AB The authors report the application of direct target-accelerated combinatorial synthesis (TACS) of vancomycin dimers for the identification of ligands with the highest affinity for vancomycin's receptor, D-Ala-D-Ala. For example, solid- and solution-phase combinatorial chemical

were

used to synthesize a library of vancomycin substrates, from which a set of monomers I [$n = 2-4$; $X = \text{SCOMe}$, CH:CH_2 ; $R = \text{H}$, $\text{D}-(\text{NMe})\text{Leu}$, $\beta\text{-Ala}$, L-Asn , etc.] were chosen for the target-accelerated dimerization step. I ($X = \text{SCOMe}$) was subjected to ligation by disulfide bond formation and I ($X = \text{CH:CH}_2$) was subjected to ligation by olefin metathesis in both the absence and presence of vancomycin's targets, Ac-D-Ala-D-Ala-OH and $\text{Ac-Lys(Ac)-D-Ala-D-Ala-OH}$, for which vancomycin has the greatest affinity. Here, a strong target-induced rate acceleration was observed in the presence

of these targets. Thus, target-accelerated combinatorial synthesis was performed, and from this library, several olefin metathesis dimers of I [n = 2-4; R = H, D-(NMe)Leu, β -Ala, Asn] and disulfide dimers of I [n = 2,3; R = D-(NMe)Leu] were identified, and these were, then, individually synthesized from their resp. monomers. Antibacterial activity for these dimers were reported; of them, some have potent activities against vancomycin-resistant enterococci (VRE) and vancomycin intermediate susceptible *Staphylococcus aureus* (VISA) that rival or exceed the most active compds. known today for these bacterial strains.

- ST target accelerated combinatorial synthesis vancomycin dimer library; olefin metathesis dimer vancomycin synthesis; disulfide vancomycin dimer synthesis; vancomycin dimer antibiotic activity resistant bacteria VRE VISA
- IT Peptides, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(cyclic; target-accelerated combinatorial synthesis of vancomycin dimers as highly potent antibiotics effective against vancomycin-resistant bacteria)
- IT Antibiotics
(macrolide; target-accelerated combinatorial synthesis of vancomycin dimers as highly potent antibiotics effective against vancomycin-resistant bacteria)
- IT Antibiotic resistance
Combinatorial library
(target-accelerated combinatorial synthesis of vancomycin dimers as highly potent antibiotics effective against vancomycin-resistant bacteria)
- IT Combinatorial chemistry
(target-accelerated; preparation of vancomycin substrates for the target-accelerated combinatorial synthesis of vancomycin dimers)
- IT 19993-26-1 24570-39-6
RL: NUU (Other use, unclassified); USES (Uses)
(as the "target" in the target-accelerated combinatorial synthesis of vancomycin dimers)
- IT 321361-97-1P 321361-99-3P 321362-01-0P 321362-03-2P 321362-05-4P
321362-07-6P 321362-09-8P 321362-11-2P 321362-13-4P
321362-15-6P 321362-17-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of vancomycin substrates for the target-accelerated combinatorial synthesis of vancomycin dimers)
- IT 60-54-8, Tetracycline 1404-90-6, Vancomycin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(target-accelerated combinatorial synthesis of vancomycin dimers as highly potent antibiotics effective against vancomycin-resistant bacteria)
- IT 321361-73-3P 321361-75-5P 321361-77-7P 321361-79-9P 321361-81-3P
321361-83-5P 321361-85-7P 321361-87-9P 321361-89-1P 321361-91-5P
321361-93-7P 321361-95-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(target-accelerated combinatorial synthesis of vancomycin dimers as highly potent antibiotics effective against vancomycin-resistant bacteria)

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

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- (31) Williams, D; Angew Chem 1999, V111, P1264
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
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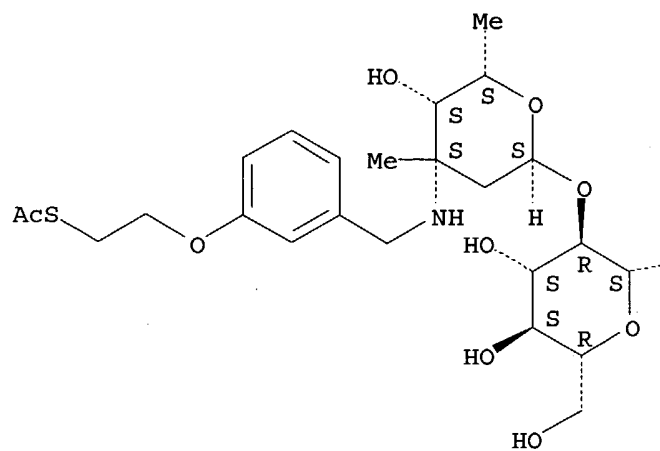
(preparation of vancomycin substrates for the target-accelerated
combinatorial synthesis of vancomycin dimers)

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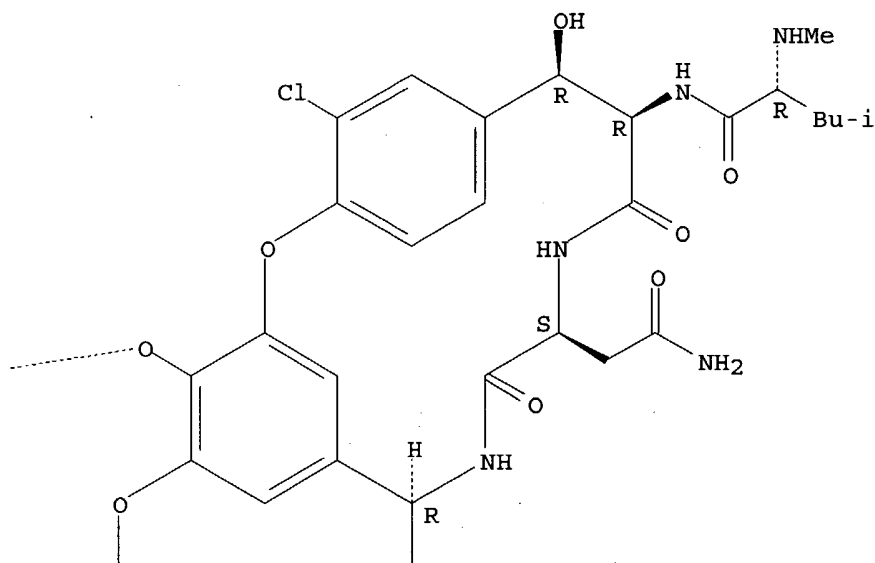
CN Vancomycin, N3'''-[[3-[2-(acetylthio)ethoxy]phenyl]methyl]- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

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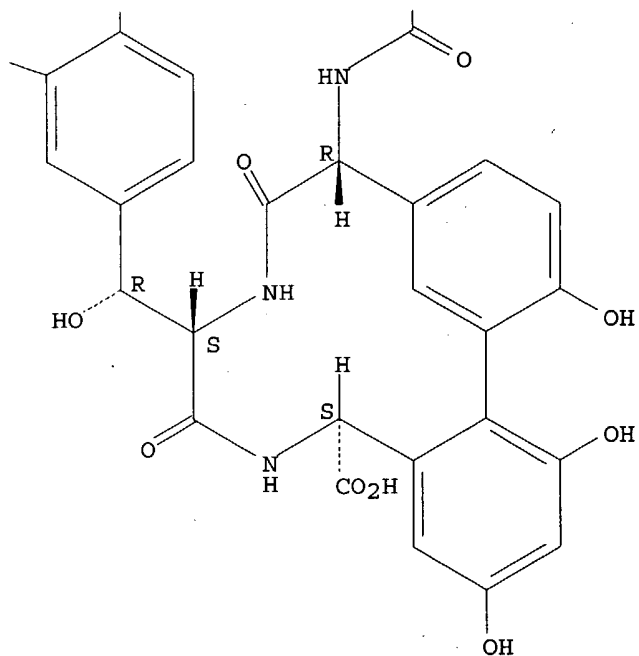
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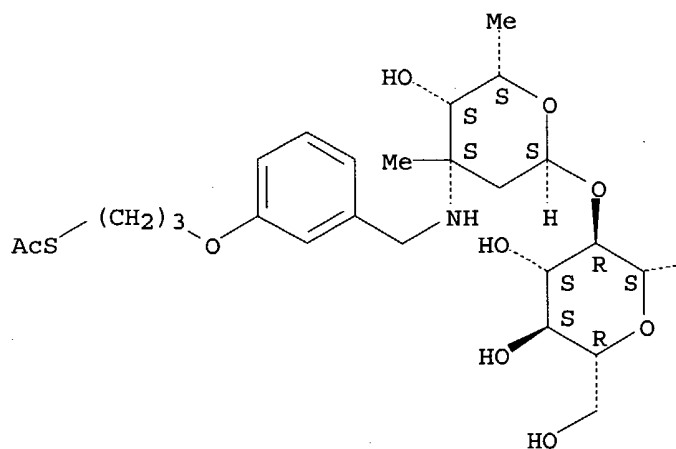


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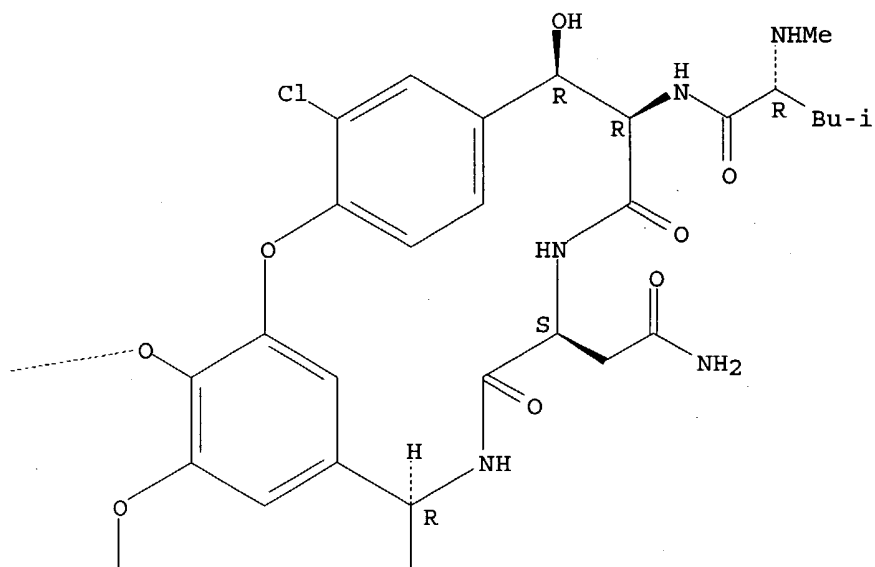
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INDEX NAME)

Absolute stereochemistry.

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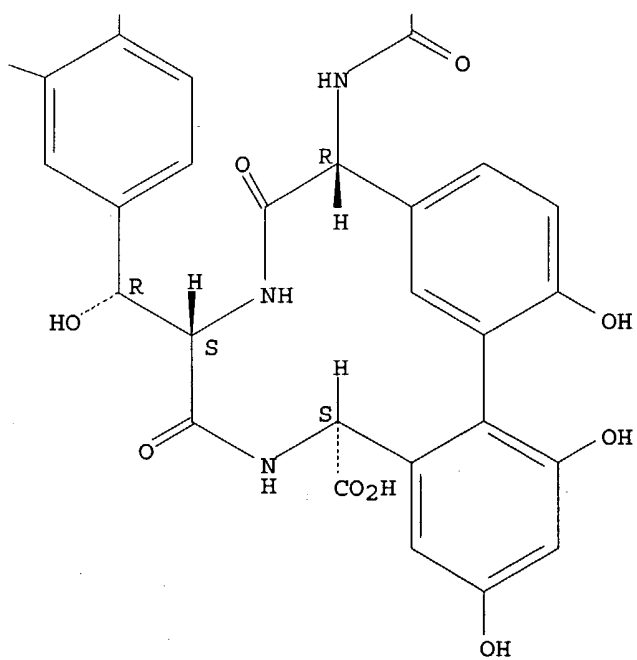
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